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LARGE ANGLE SCATTERING OF  $H^+$  AND  $H_2^+$  BY  
ARGON

by

Everrette Verne Snotherly



# United States Naval Postgraduate School



## THESIS

LARGE ANGLE SCATTERING OF  $H^+$  AND  $H_2^+$

BY ARGON

by

Everrette Verne Snotherly, Jr.

October 1969

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Large Angle Scattering of  $H^+$  and  $H_2^+$  by Argon

by

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Submitted in partial fulfillment of the  
requirements for the degree of

MASTER OF SCIENCE IN PHYSICS

from the

NAVAL POSTGRADUATE SCHOOL  
October 1969

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# ABSTRACT

The elastic differential scattering cross sections for  $\underline{\text{H}}^+$ ,  $\underline{\text{H}}_2^+ + \text{Ar} \rightarrow \underline{\text{H}}^+$ ,  $\underline{\text{H}}_2^+ + \text{Ar}$  were measured for angles of  $39^\circ$  to  $50^\circ$  with incident lab energy of 100 eV. The apparatus utilized the properties of axially symmetric, non-uniform magnetic fields (large thin solenoid) to focus all scattered ions with vector momentum  $\vec{p}$  within  $\Delta\vec{p}$  onto a detector placed down the magnetic axis. Thus, the solid angle was increased by a factor of about 300 over conventional methods with comparable resolution in  $\Delta\theta$  (about  $1^\circ$ ). A typical value for  $\sigma_{\text{H}^+}(43^\circ)$  is  $8.2 \times 10^{-18} \text{ cm}^2$ . The  $\text{H}^+$  data was compared with data of Magnuson, et.al., via a scaling law and was in excellent agreement. A typical value for  $\sigma_{\text{H}_2^+}(43^\circ)$  is  $2.4 \times 10^{-20} \text{ cm}^2$ . A simple refinement of a classical model for  $\text{H}_2^+$  scattering by Feist relates these cross sections by  $\sigma_{\text{H}_2^+}(\theta) = P \sigma_{\text{H}^+}(\theta) \simeq \frac{4D}{\pi\ell^2 E_0} [\sigma_{\text{H}^+}(\theta)]^2$  where  $P$  is an orientation factor,  $D$  the binding energy, and  $\ell$  the internuclear separation. This expression relates the cross sections to within the accuracy of the experiment thus verifying the classical approximations.

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I am grateful to Dr. G.D. Magnuson of the University of Virginia for relaying his data from a similar experiment. This greatly assisted in analyzing our own data.



## I. INTRODUCTION

Atomic processes such as the scattering of complex ions by heavy atoms are properly described by quantum mechanics. Unfortunately, for a many-body problem the mathematics becomes untractable. In order to produce useful solutions approximations must be introduced. One class of approximations involves the use of semi-classical models of the collision process. By sacrificing rigor, useful solutions are obtained that still provide insight into the physical process involved.

The classical model investigated here is used to calculate the differential scattering cross section of the  $H_2^+$  ion by a spherically symmetric potential. The theory was developed by Feist [1] based on the earlier work of Bates, Cook, and Smith [2] as follows. First, calculate the differential scattering cross section of a single proton from a spherically symmetric potential. Then calculate the probability that the second proton is oriented with respect to the first such that the  $H_2^+$  molecule is not disrupted by the collision. The differential scattering cross section for  $H_2^+$  is the product of this orientation probability times the cross section for the single proton.

The purpose of the experiment reported here was to test the theory as developed by Feist. This was done by measuring the differential scattering cross section of  $H^+$  by Argon and

$H_2^+$  by Argon at incident energies of 100 eV and laboratory angles from  $39^\circ$  to  $49^\circ$ . Thus, the orientation probability was determined experimentally and compared with Feist's calculation.



## II. THEORY

### A. THE MODEL

This classical model is applicable to the scattering of the  $H_2^+$  ion over a range of incident energies  $E_0$  (in laboratory coordinates) by a spherically symmetric potential such as heavy noble gas atoms. The reaction studied was  $\underline{H_2^+} + Ar \rightarrow \underline{H_2^+} + Ar$  where the underline indicates the fast particle in laboratory coordinates. The two protons of the  $H_2^+$  ion have an equilibrium separation in the ground state of 1.06 angstroms and a disassociation energy of 2.648 eV. The lower energy limit where this model could no longer be expected to apply would be where the incident ion energy becomes comparable with the ion binding energy. This requires that  $E_0 \gg 2.648$  eV or  $E_0 \gtrsim 30$  eV. The upper energy limit where this model could no longer be expected to apply is governed by the uncertainty principle. In this application it is required that the de Broglie wavelength be much less than the distance of closest approach or  $r_0 \gg \lambda_D = \frac{h}{mv_0}$  which may be written as  $r_0 \geq \frac{10h}{\sqrt{2mE_0}}$ . Now  $r_0$  may be further related to  $E_0$  by considering a head-on collision with the shielded coulomb potential for Argon (this potential is discussed in Section II B, and Appendix A). Considering only the dominant term of the potential one can write

$$E_0 = \frac{Ze^2}{r_0} A e^{-\alpha r_0}$$

where  $A$  and  $\alpha$  are parameters of the potential. Substituting



values for the constants one obtains

$$E_o = 14.6 \frac{1}{r_o^2}$$

$$\text{and } E_o = 411 \frac{1}{r_o} e^{-1.68 r_o}$$

with  $E_o$  in units of eV and  $r_o$  in units of Bohr radii. The value of  $E_o$  that satisfies these equations is  $E_o = 1.13 \times 10^4$  eV. This shows that a classical model for the scattering of  $H_2^+$  should be valid for incident energies up to about 10 KeV.

In a scattering event the  $H_2^+$  ion may be disrupted due to the following two effects. First, consider the two protons approaching a spherically symmetric potential with the same impact parameter,  $b$ . Using the concept of an impulse approximation, consider each proton-target collision separately, yielding a description in terms of two two-body collisions. Due to the spherical symmetry each proton scattered is confined to a plane defined by the scattering axis and a line from the scattering center to the proton. The angular difference between the scattering planes,  $\Delta\theta$  will result in a difference in velocities of the two protons after scattering such that their relative energy may be greater than the binding energy and the  $H_2^+$  ion will be disrupted. Figure 1 illustrates this process.

Second, consider the protons oriented such that they will be scattered in the same plane but with different impact parameters.

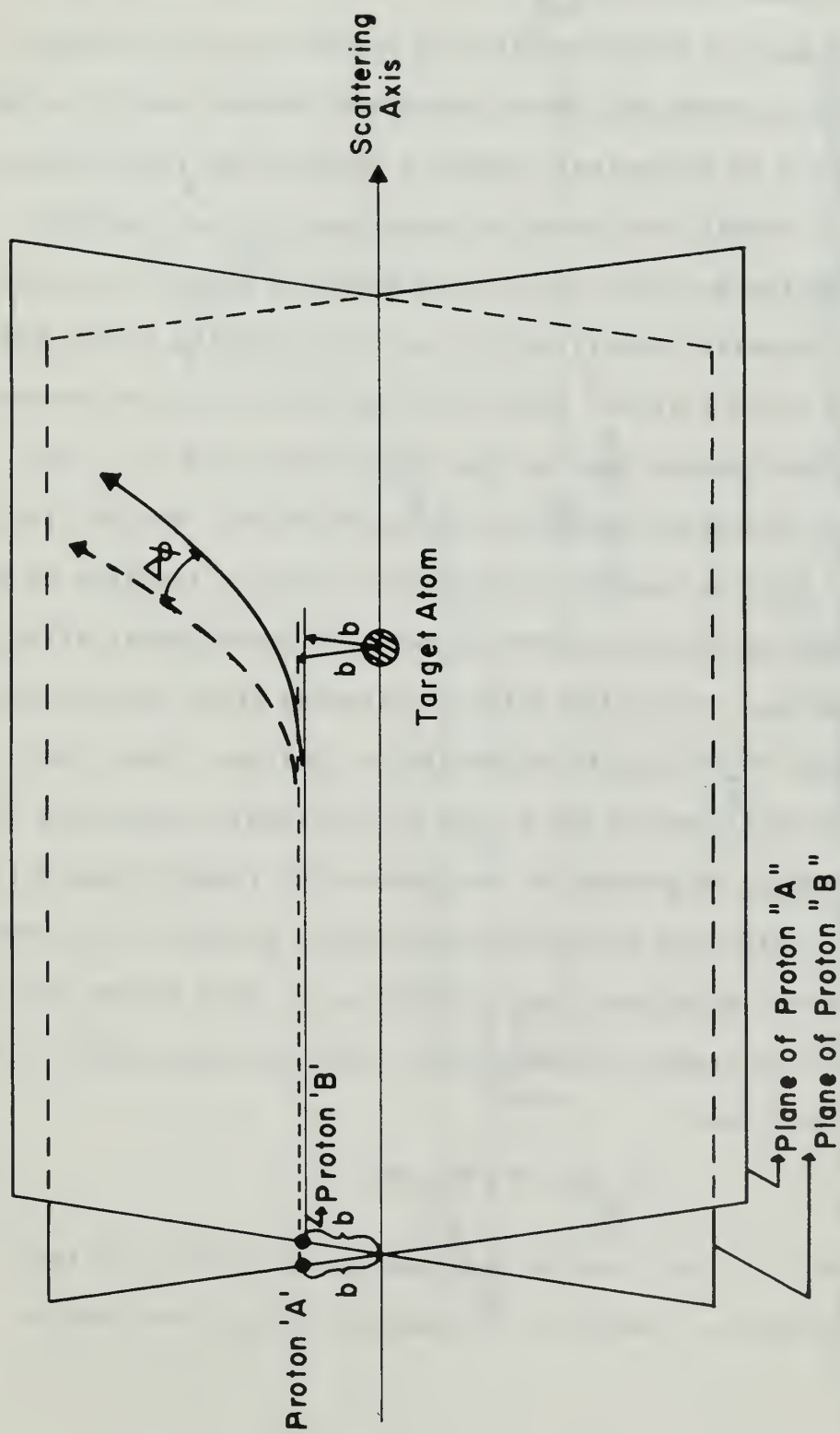


Figure 1. Protons with same impact parameter but different scattering planes.

This will result in a difference in scattering angle  $\Delta\theta$  and therefore again a relative velocity between the two protons. The relative energy may again exceed the binding energy so that the ion will be disrupted. Figure 2 illustrates this process.

In the actual case these two processes are not separable and disruption may occur due to the combined effect of  $\Delta\phi$  and  $\Delta\theta$ . The necessary condition for the ion remaining intact after collision is  $D > \frac{1}{2} \mu (\Delta V)^2$  where  $D$  is the disassociation energy,  $\mu = M_p/2$  the reduced mass of the two protons, and  $\Delta V$  is the difference in velocities due to both  $\Delta\phi$  and  $\Delta\theta$ . Whether the  $H_2^+ + Ar \rightarrow H_2^+ + Ar$  reaction will occur is then a function of the orientation of the two protons before (or equivalently after) the collision. The differential scattering cross section for the  $H_2^+$  ion,  $\sigma_{H_2^+}(\theta)$  may be calculated as follows. For  $E \gg D$  treat the collision of the  $H_2^+$  ion as two events consisting of the scattering of proton "A" and proton "B" (impulse approximation). Calculate the differential cross section for proton "A",  $\sigma_H(\theta)$ . Calculate the probability,  $P$ , that proton "B" is oriented with respect to proton "A" such that  $D > \frac{1}{2} \mu (\Delta V)^2$ . It then follows that

$$\sigma_{H_2^+}(\theta) = P \sigma_H(\theta). \quad (1)$$

The electron is not treated as a scattered particle in this model but may be thought of as simply providing the binding energy.

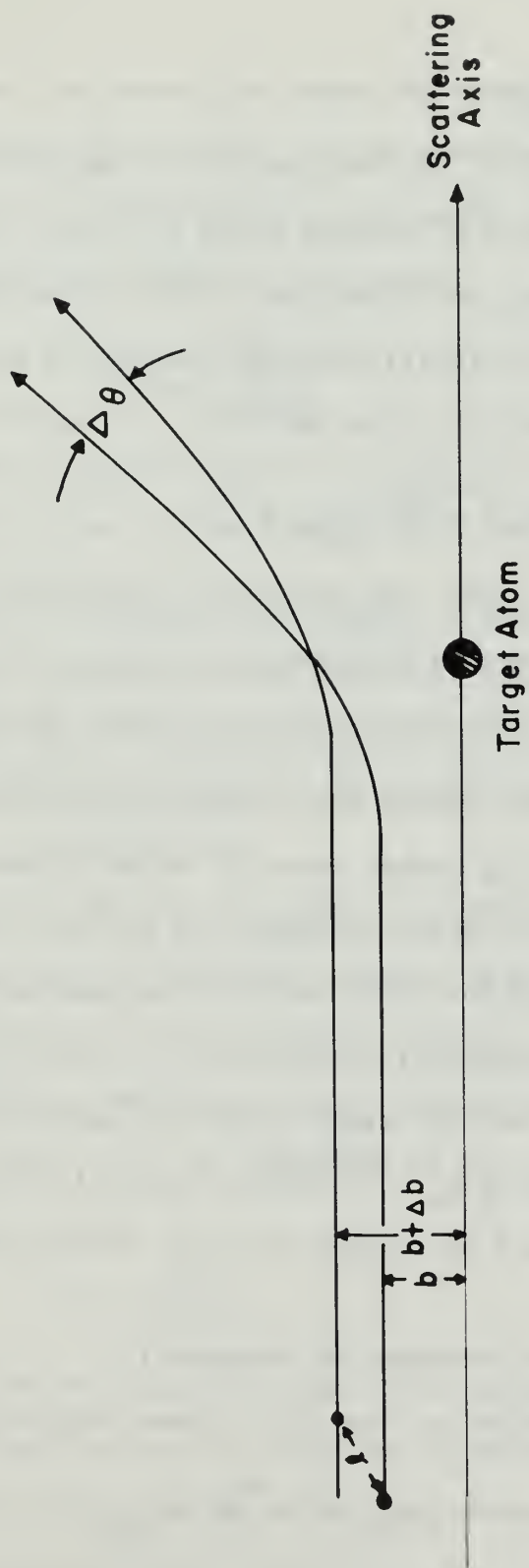


Figure 2. Protons with the same scattering plane but different impact parameters.

## B. CALCULATION OF $\sigma_{H^+}(\theta)$

The calculation of  $\sigma_{H^+}(\theta)$  was done on an IBM 360-67 digital computer using a program written by Feist [2]. The program utilizes standard numerical techniques to solve the classical differential scattering equations. The potentials used are shielded coulomb potentials from Byatt [3] of the form

$$V(r) = \frac{Ze^2}{r} \left( \sum_n C_n e^{-b_n r} \right)$$

with  $\sum_n C_n = 1$  but  $C_n$  and  $b_n$  otherwise adjustable. Byatt lists two potentials for Argon, one with and one without correction for polarization. The two potentials yielded cross sections for  $H^+$  that were within 13% of each other for an incident energy of 100 eV and scattering angles from  $38^\circ$  to  $50^\circ$  (laboratory coordinates). Due to the close agreement of the two potentials, only the one corrected for polarization is presented here.

Byatt indicates the potentials should be accurate to within 5% for  $\sum_n C_n e^{-b_n r} > .01$ . For the region where the potentials were used it was noted that  $\sum_n C_n e^{-b_n r} > .052$ . Thus it was felt that these potentials should be satisfactory for calculating  $\sigma_{H^+}(\theta)$ .

## C. CALCULATION OF THE ORIENTATION PROBABILITY

The energy criterion for the  $H_2^+$  ion remaining intact may be put as

$$D = \frac{\mu}{2} (\Delta V_{\max})^2 = \frac{M_D}{4} (\Delta V_{\max})^2$$

$$\text{or} \quad \Delta V_{\max} = \left[ \frac{4D}{M_D} \right]^{\frac{1}{2}}. \quad (2)$$



Considering the case where the target mass is much greater than the mass of the  $H_2^+$  ion, the  $H_2^+$  ion has energy after collision  $E_o = M_p V_o^2$  both in the laboratory and center of mass systems. Substituting this into equation (2) gives

$$\Delta V_{\max} = \left[ \frac{4D}{E_o} \right]^{\frac{1}{2}} V_o .$$

Now it was shown in Section II A, that  $\Delta V_{\max} = f(b, \Delta b, \Delta\emptyset)$ . Therefore, for a fixed incident energy and impact parameter, there exists a function  $g$  such that  $\Delta\emptyset = g(\Delta b)$ . This defines a closed curve in a plane perpendicular to the scattering axis that proton "B" must pass through in order for the ion to remain intact. The area enclosed by the  $\Delta\emptyset = g(\Delta b)$  curve is designated by  $S$ .

The axis of the  $H_2^+$  ion is randomly oriented with proton "B" having no preferred position with respect to proton "A". The location of proton "B" will therefore define a sphere about proton "A" of radius  $\ell$ , the internuclear separation. The orientation probability is then given by the ratio of  $S$  to one-half the area of this sphere

$$P = \frac{S}{2\pi\ell^2} . \quad (3)$$

The justification for using the area of a hemisphere in the denominator of equation (3) is that the "other half" is redundant. No exact solution has been found for equation (3) and the following approximations were made.

First, it has been assumed that the target is infinitely heavy so that the speed of the  $H_2^+$  ion is unchanged by the collision. For the reaction studied experimentally, this is valid in that  $M_{H_2^+} = 2.032$  amu and  $M_{Ar} = 39.948$  amu. For example, a 100 eV  $H_2^+$  ion scattered at  $45^\circ$  has an initial speed of  $9.80 \times 10^4$  m/sec and a final speed of  $9.75 \times 10^4$  m/sec. It is further assumed that the two protons will both have this same speed after collision and that disruption will occur due to difference in direction only. Feist [1] showed that the disruptive effect of the difference in the magnitudes of velocities of the two protons is much less than the disruptive effect of their difference in direction. For the case where  $\Delta\theta = 0$ , and assuming  $\Delta\theta$  is small,  $\Delta V_{\max} = V_o [\Delta\theta_{\max}]_{\Delta\theta = 0}$ . Using equation (2) this becomes

$$[\Delta\theta_{\max}]_{\Delta\theta = 0} = \left[ \frac{4D}{E_o} \right]^{1/2} . \quad (4)$$

Figure 3a illustrates this case. For the case where  $\Delta\theta = 0$  (or equivalently  $\Delta b = 0$ ) and assuming  $\Delta\theta$  is small,

$\Delta V_{\max} = V_o \sin \theta [\Delta\theta_{\max}]_{\Delta b = 0}$ . Using equation (2) this becomes

$$[\Delta\theta_{\max}]_{\Delta b = 0} = \left[ \frac{4D}{E_o} \right]^{1/2} \frac{1}{\sin \theta} . \quad (5)$$

Figure 3b illustrates this case. Using the classical definition for differential scattering  $|2\pi b db| = |\sigma_{H^+}(\theta) 2\pi \sin \theta d\theta|$ , it is seen that

$$|\Delta b_{\max}|_{\Delta\theta = 0} = \frac{\sigma_{H^+}(\theta) \sin \theta}{b} [\Delta\theta_{\max}]_{\Delta\theta = 0} ,$$

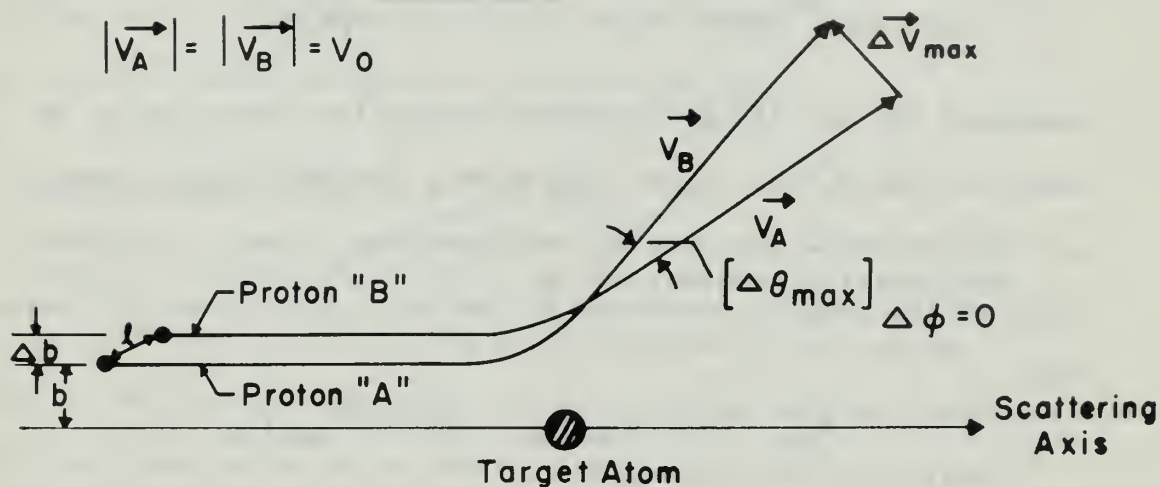


Figure 3.a. Proton velocity difference due to difference in impact parameter.

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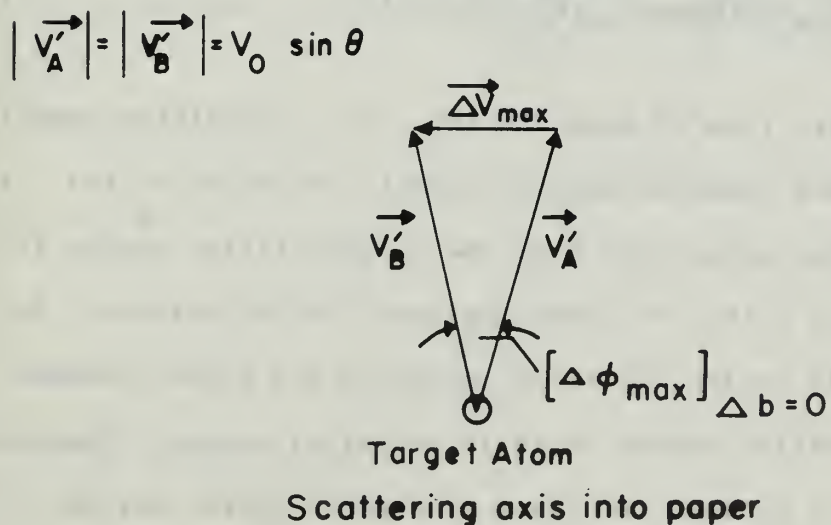


Figure 3. b. Proton velocity difference due to difference in scattering plane.



which, upon combining with equation (4) becomes

$$|\Delta b_{\max}|_{\Delta\theta = 0} = \frac{\sigma_{H^+}(\theta) \sin \theta}{b} \left[ \frac{4D}{E_0} \right]^{\frac{1}{2}}. \quad (6)$$

Equations (5) and (6) give maximum values for either  $\Delta b$  or  $\Delta\theta$  such that the  $H_2^+$  ion is not disrupted. The  $\Delta\theta = g(\Delta b)$  curve must therefore be enclosed by these maximum values. An upper bound on the area,  $S$ , enclosed by the  $\Delta\theta = g(\Delta b)$  curve is therefore

$$S_{\max} = [2(\Delta b_{\max})_{\Delta\theta = 0}] [2b(\Delta\theta_{\max})_{\Delta b = 0}].$$

Substituting equations (5) and (6) into the above and using equation (3) an upper bound on the orientation probability is found to be

$$P_{\max} = 8 \frac{D}{E_0} \frac{\sigma_{H^+}(\theta)}{\pi \ell^2} \quad (7)$$

$$\text{and } \left[ \sigma_{H_2^+}(\theta) \right]_{\max} = \frac{8D}{\pi \ell^2 E_0} [\sigma_{H^+}(\theta)]^2. \quad (8)$$

Due to the simple form of equation (8), it is calculated numerically in the same computer program used to calculate  $\sigma_{H^+}(\theta)$ . It should be further noted that  $D$  is the disassociation energy for ground state and  $\ell$  the corresponding equilibrium distance. Excited electronic states for the  $H_2^+$  molecule are either unbound or have very shallow minima in their potential curves. Therefore, if the  $H_2^+$  ion is excited to higher electronic states during the collision process it is almost certain to be disrupted due to

velocity differences after the collision. If the  $H_2^+$  ion is excited to higher vibrational levels, then  $D$  would be decreased and  $\ell$  increased. The molecule could still remain intact but would have a smaller value of  $P$  and hence  $\sigma_{H_2^+}(\theta)$ .

#### D. COMPUTER CALCULATION OF $\sigma_{H^+}(\theta)$ AND $\sigma_{H_2^+}(\theta)$

Figure 4 displays the results of the computer calculations for the differential scattering cross sections. One set of curves is for the  $H^+ + Ar \rightarrow H^+ + Ar$  reaction at incident energies of 100, 300, and 500 electron-volts. The second set of curves is for the  $H_2^+ + Ar \rightarrow H_2^+ + Ar$  reaction also at incident energies of 100, 300, and 500 electron-volts. The  $H_2^+$  curves were computed using equation (8) and represent a predicted upper limit on the scattering cross section.

It is noted that all of the curves are monotonically decreasing functions of scattering angle and reflect no atomic structure.

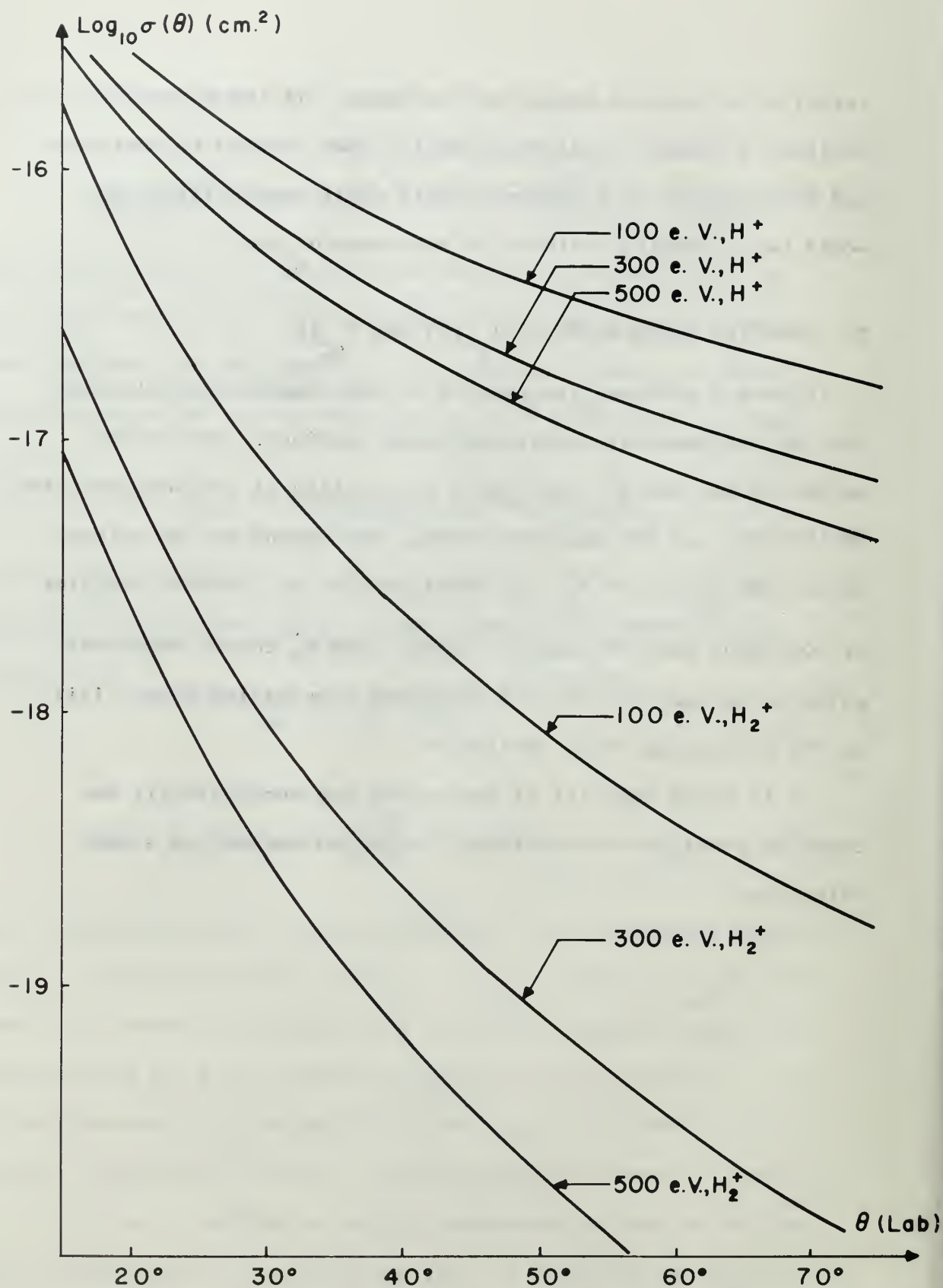


Figure 4. Log of scattering cross section vs. scattering angle for  $\text{H}^+ + \text{Ar} \rightarrow \text{H}^+ + \text{Ar}$  and  $\text{H}_2^+ + \text{Ar} \rightarrow \text{H}_2^+ + \text{Ar}$ .

### III. EXPERIMENTAL APPARATUS

#### A. GENERAL DESCRIPTION.

The experimental apparatus used to measure the cross sections for the  $\underline{\text{H}}^+$ ,  $\underline{\text{H}}_2^+ + \text{Ar} \rightarrow \underline{\text{H}}^+$ ,  $\underline{\text{H}}_2^+ + \text{Ar}$  reactions is discussed in detail by Bush [4]. An overall schematic of the apparatus is shown in Fig. 5. The operation of the apparatus was as follows. Three species of hydrogen ions ( $\text{H}^+$ ,  $\text{H}_2^+$ ,  $\text{H}_3^+$ ) were produced in the duoplasmatron ion source and were accelerated electrostatically to the desired energy. The ions entered a mass analyzer where the desired ion species was bent through a  $45^\circ$  angle to travel down the geometric axis of the apparatus. The selected beam was focused and entered the scattering cell where the target gas, in this case Argon, was contained. The scattering cell was centered in a large focusing magnet that produced a known non-uniform but axially symmetric magnetic field. The trajectory of an ion with a given vector momentum could then be calculated and the detector was appropriately placed to collect this ion. Due to the finite detector size, ions scattered within a finite  $\Delta\theta$  (on the order of  $1^\circ$ ) were also detected. It is further noted that essentially all the ions scattered at an angle  $\theta$  were collected regardless of their azimuthal angle of departure. Cross section measurements at different scattering angles could be made in two ways. Either the detector could be fixed on the magnetic/geometric axis and the focusing magnet current varied to select



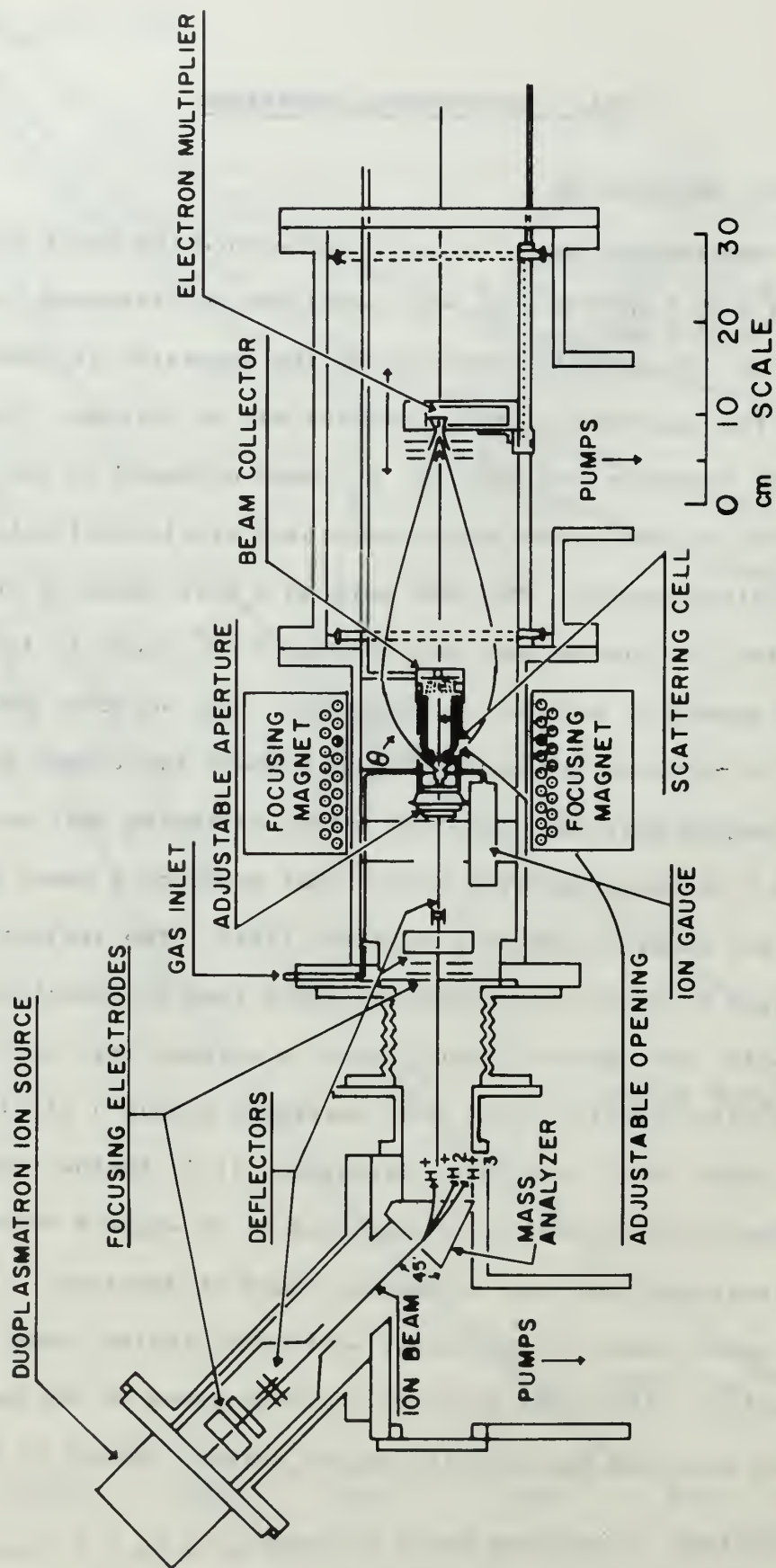


FIGURE 5. SCHEMATIC OF THE EXPERIMENTAL APPARATUS.

the desired scattering angles, or the focusing magnet current could be fixed and the detector moved along the magnetic/geometric axis to select the desired scattering angles. In this experiment, the latter method was used. The detector system consisted of a magnetic electron multiplier whose output was fed into an electrometer. The entire system was maintained at a vacuum on the order of  $10^{-5}$  torr during operation by two diffusion pumps.

#### B. THE DUOPLASMATRON ION SOURCE.

The duoplasmatron ion source was constructed and described in detail by Carter [5]. Figures 6 and 7 display the construction of the source and the circuit diagram for its operation. The operation of the source basically consisted of maintaining the plasma discharge in the Z-electrode cavity and extracting ions at the desired energy by placing this potential on the anode. Focusing the extracted beam was accomplished by an electro-magnet surrounding the Z-electrode cavity and a conventional Einzel lens and deflector stack.

To increase the beam intensity an acceleration-deceleration system was utilized. This consisted of extending the extraction lens,  $L_1$ , to enclose the entire focusing stack. This enclosure was called the "sock". (See Fig. 7.) By floating the sock at a negative potential  $V$  (typically -500 volts) and by increasing the potentials of the interior lenses and deflectors by the same amount, the extracted ions transversed this region with an energy

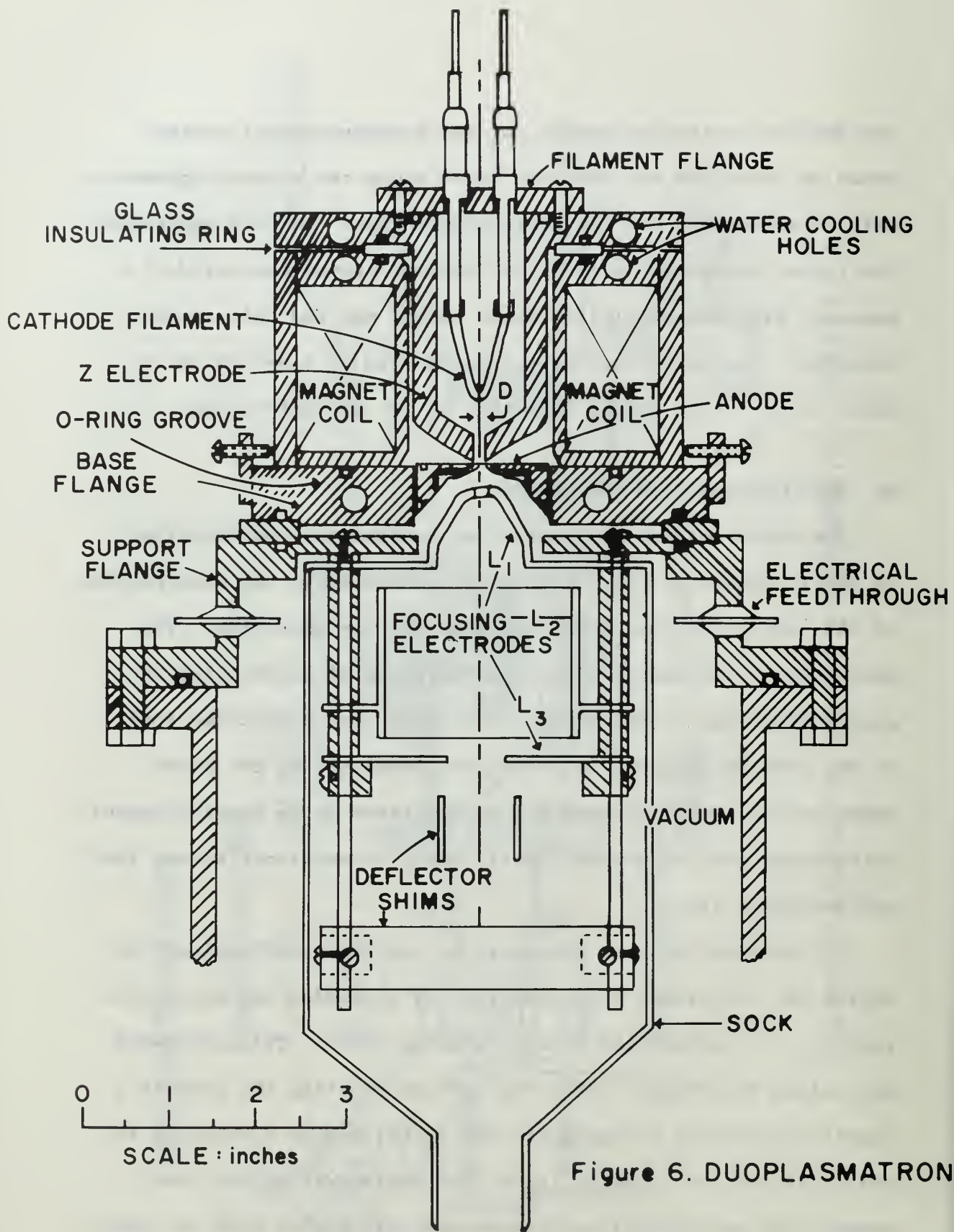


Figure 6. DUOPLASMATRON



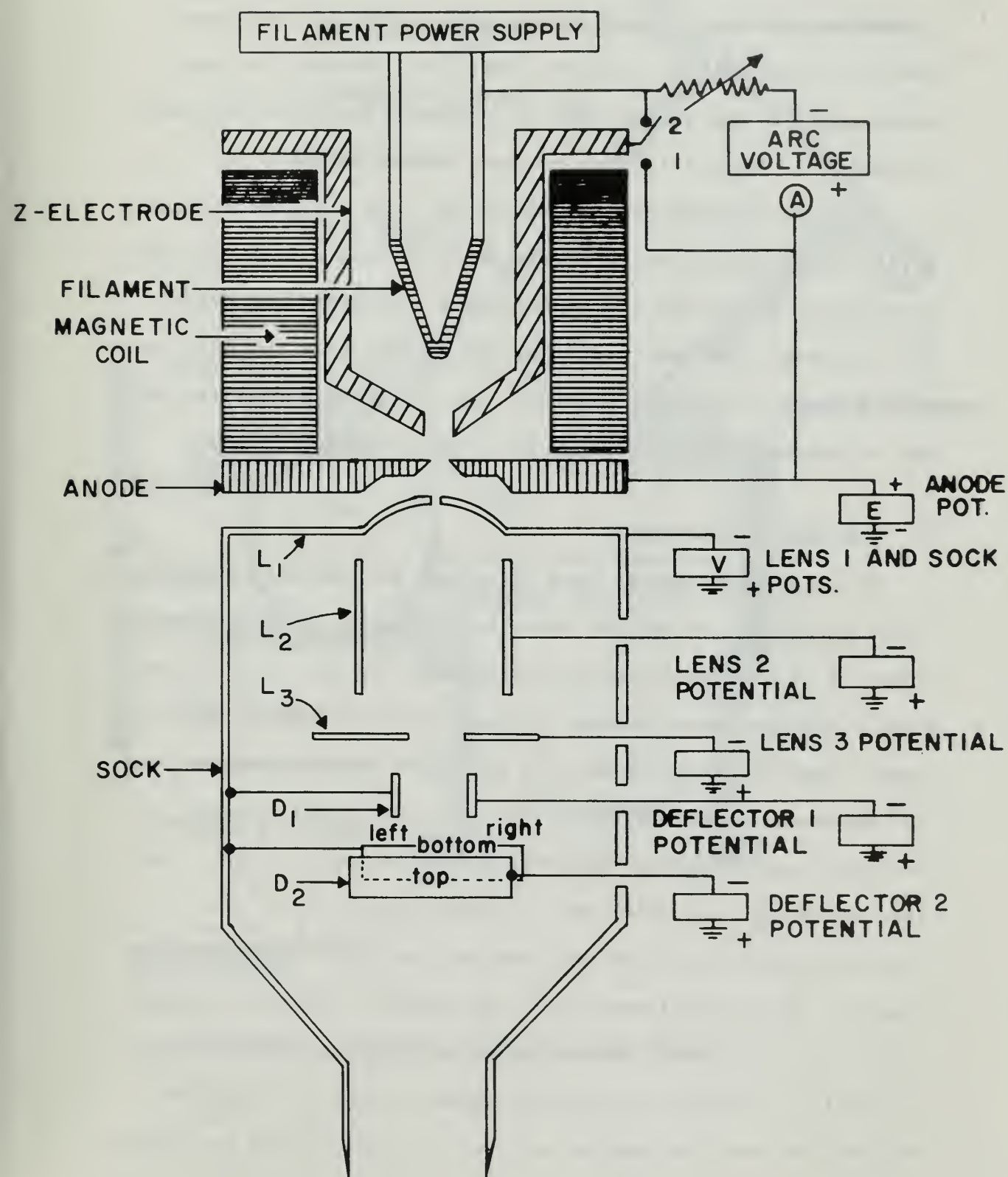


FIGURE 7.  
CIRCUIT DIAGRAM FOR DUOPLASMATRON



$(E + V)e$ , yielding a higher space charge limit for the beam density. Upon exiting from the sock, the hydrogen ions were decelerated to energy  $E_e$ . This arrangement increased the beam intensity at the scattering cell by a factor of about 40.

A typical maximum beam intensity for mass analyzed protons of 100 eV delivered to the scattering cell with 0.5 cm entrance aperture at 80 cm from the source was  $1 \times 10^{-7}$  amperes. For  $H_2^+$  ions under the same conditions the maximum beam intensity was on the order of  $2 \times 10^{-7}$  amperes. The energy spread of the beam was estimated to be about 2 eV for a 100 eV beam.

### C. THE MASS SPECTROMETER.

The mass spectrometer used to select the desired ion was constructed, calibrated and described in detail by Strohsahl [6]. Figure 8 is a schematic of its arrangement in the overall apparatus. The mass spectrometer utilized an electromagnet to produce a magnetic field of up to 4 kilogauss confined between two  $40^\circ$  wedge-shaped pole pieces. This was sufficient to mass analyze atomic masses up to 40 with energies up to 1 KeV. The resolution ( $\frac{m}{\Delta m}$ ) was about 40. A bending angle of  $45^\circ$  was utilized and this altered the selected ion beam trajectory from the axis of the duoplasmatron to the geometric axis of the main scattering apparatus. Operation of the mass analyzer consisted of merely of setting the correct magnet current to focus the desired ion into the scattering cell. The pole faces and region

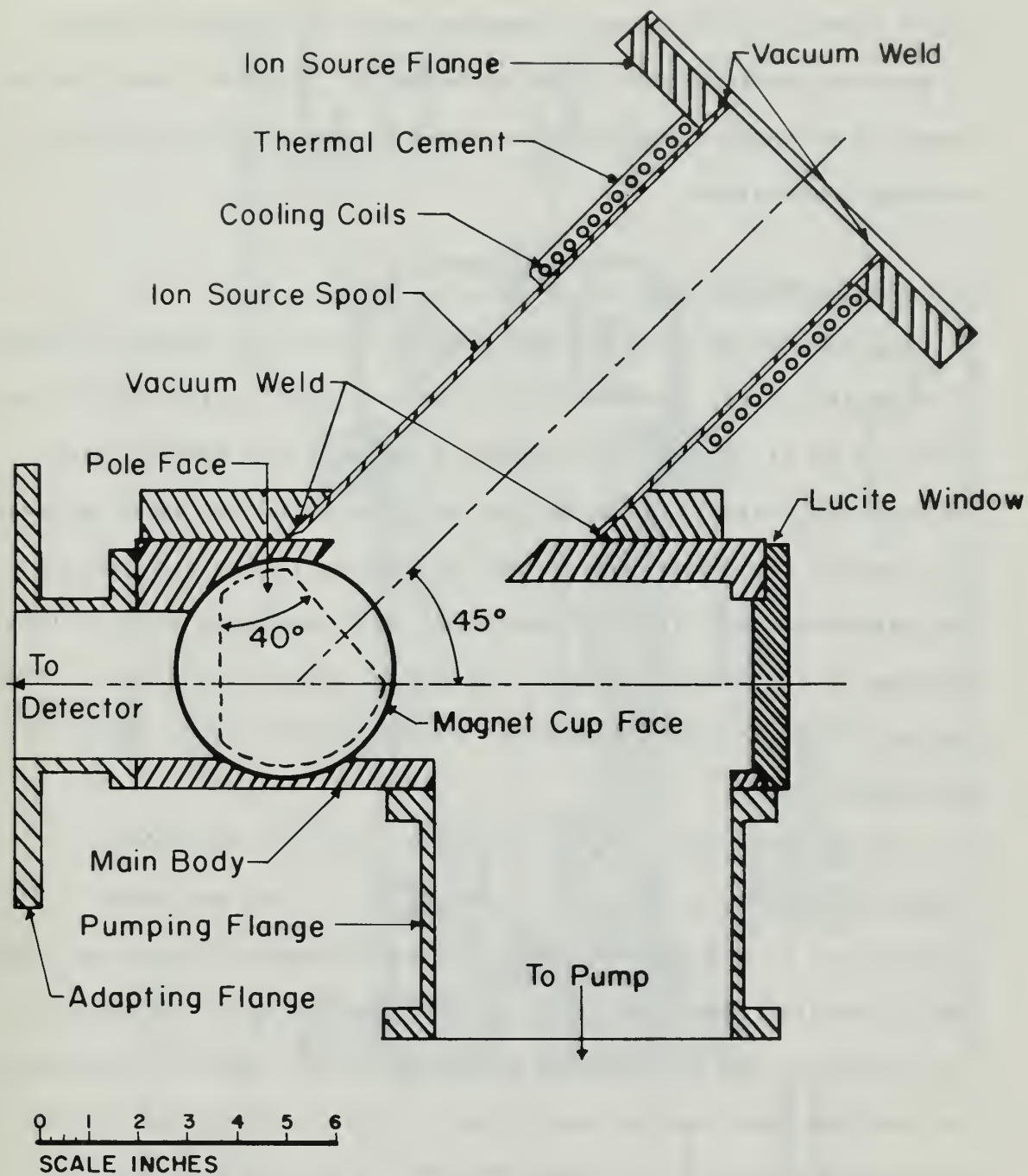


Figure 8. Schematic of Mass Spectrometer.

where undesired species were "dumped" were coated with aquadag to prevent static charges from building up. Even so, this region required thorough cleaning after about 20 hours of duoplasmatron-analyzer operations.

#### D. THE SCATTERING CELL.

The scattering cell was designed by Bush [4]. Figure 9 shows a schematic of its construction. The functions of the scattering cell are to (1) allow the collimated incident ion beam to pass through the scattering region and be measured by the beam collector, (2) contain the target gas in the scattering region and measure its pressure, and (3) allow scattered ions to escape over as large a range of scattering angle and azimuthal angle as possible. The design of the scattering cell was a compromise between these requirements.

The incident beam enters the scattering cell through an adjustable aperture (diameter from 0.1 to 1.0 cm) which was usually set at 0.5 cm. The beam passed through the front section which contains the scattering region. Now the great majority of the incident ions will not be scattered at all and will continue on into the rear section where they are collected either by the rear section wall or the beam collector. The incident beam was measured by two Keithly Model 410 Micro-Microammeters. The beam collector, which collects about 90% of the beam, had three grids that prevented slow ions from being collected and suppressed secondary electron emission. The beam collector assembly could be swung off axis allowing a clear path through the scattering cell for system alignment and detector calibration.

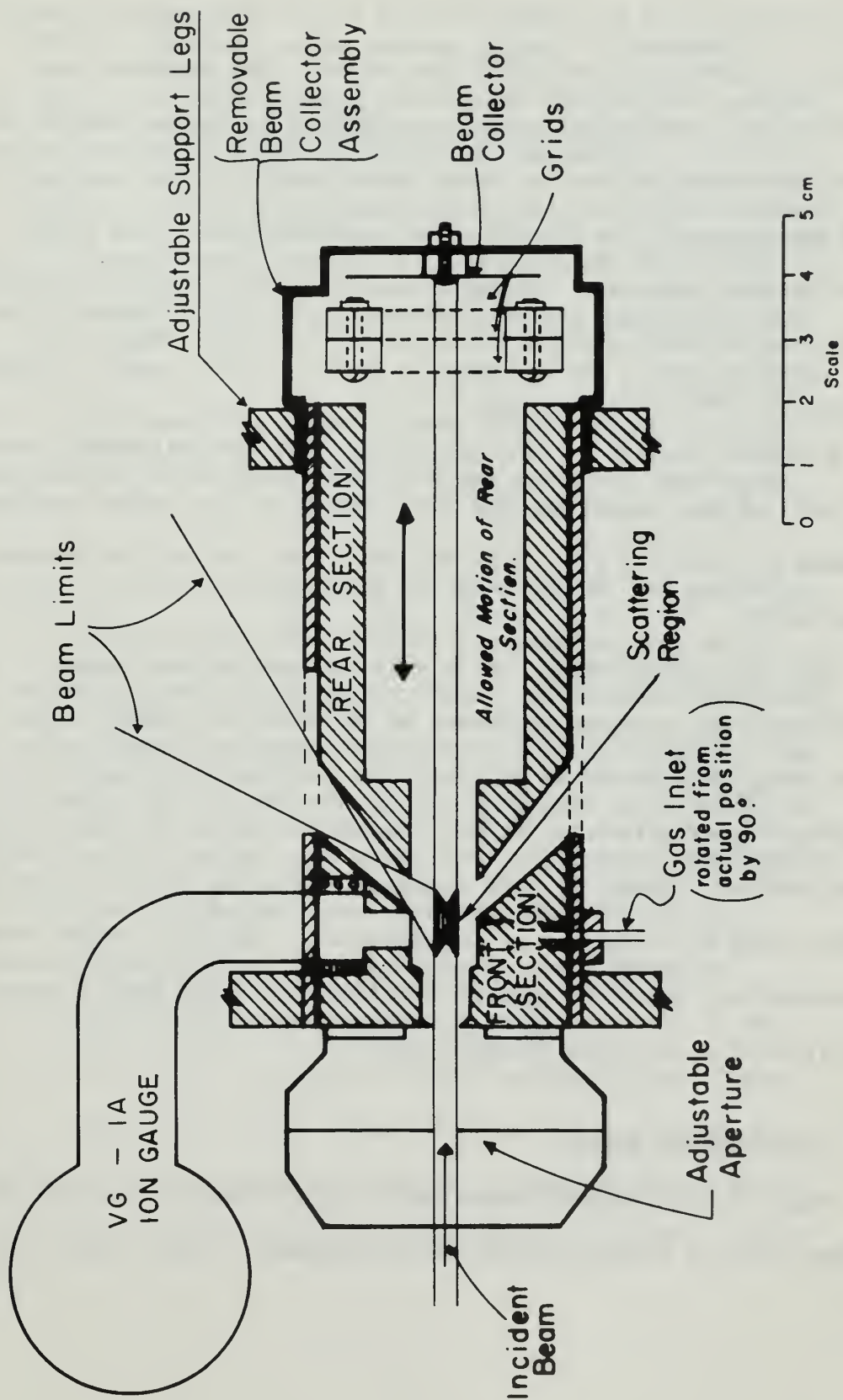


Figure 9. The Scattering Cell and Beam Collector



The target gas was bled into the scattering region through a Granville-Phillips variable leak valve. The pressure was measured by a VG-1A ion gauge manufactured by Vacuum Industries. Since operation of the ion gauge interfered with the incident beam measurement, the pressure was measured before and after each run and averaged. Vacuum Industries lists the correction factor for Argon (relative to dry air) as 0.617. That is,

$$P_{\text{actual}} = 0.617 \times P_{\text{indicated}}$$

The rear section of the scattering cell was adjustable along the axis of the apparatus and thus regulated the target thickness between 0.1 and 0.8 cm. This was set at 0.3 cm for the present experiment.

The scattering angle limits were defined by the slope of the front and rear section shoulders of  $49^\circ$  and  $36^\circ$  respectively. This range of scattering angles could be extended somewhat by considering an effective target thickness. Bush [4] describes this process. Ideally, ions scattered into all  $360^\circ$  of azimuthal angle could be collected at the detector. However, interference by mechanical support required for the scattering cell reduced the available azimuthal angle to  $290^\circ$ .

#### E. THE FOCUSING MAGNET.

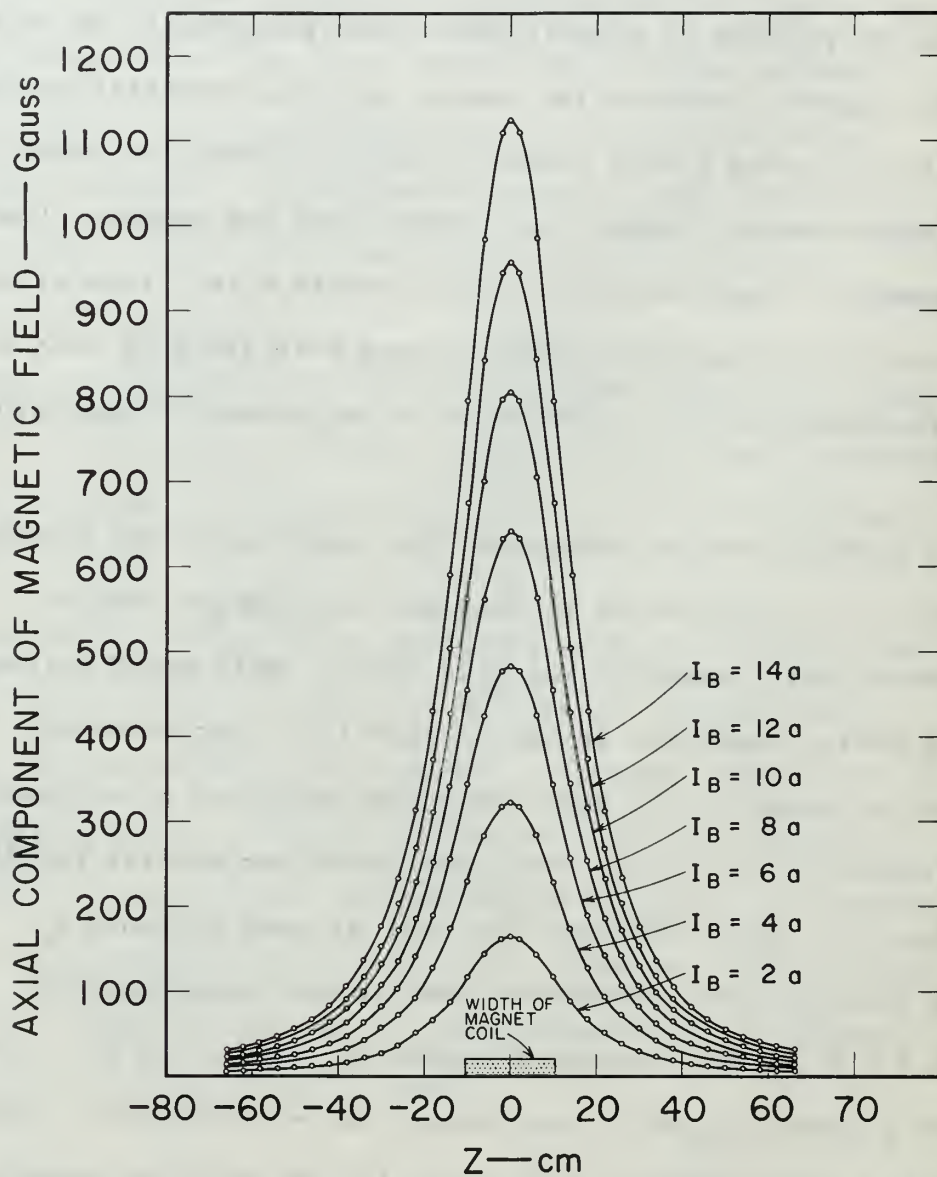
The focusing magnet consisted of five concentric spools of copper wire in a parallel-series arrangement. Each spool was

water-cooled by a  $\frac{1}{4}$  inch copper tubing jacket. A Sorenson Nobatron DCR 150-15 power supply maintained the desired current setting for periods of several hours with essentially no drift.

The magnetic field on the center axis was carefully surveyed by Kelly [7] using a Hall probe. Figure 10 shows the result of these measurements. Kelly also showed that the magnetic field was symmetric about the coil axis to within 0.1%. This allowed the axis of the apparatus to be aligned with the coil axis so that the magnetic axis coincided with the geometric apparatus axis.

In order to better understand the function of the focusing magnet, it is instructive to consider the simpler case of a uniform axially symmetric magnetic field. This would correspond to the entire apparatus being enclosed in a long solenoid. For an ion of charge  $q$  with momentum  $p$  and scattered at an angle  $\theta$  the trajectory is a helix such that after one orbital revolution the ion will again intercept the axis at some distance  $Z_0$ .

Using these boundary conditions the Lorenz force equation  $\vec{F} = q \vec{v} \times \vec{B}$  can be integrated to give  $Z_0 = \frac{2\pi}{qB} p \cos \theta$ . A detector placed at  $Z_0$  will then detect the scattered ion. (See Fig. 11.) This equation also shows the two ways of detecting scattered ions over a range of  $\theta$  and  $p$ . Either maintain  $B$  constant and vary the detector position or keep the detector fixed and vary  $B$ .



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Figure 10. Magnetic Field Strength at Various Distances Along the Magnetic Axis for Various Currents

$$B_z = B$$

$$B_r = B_\phi = 0$$

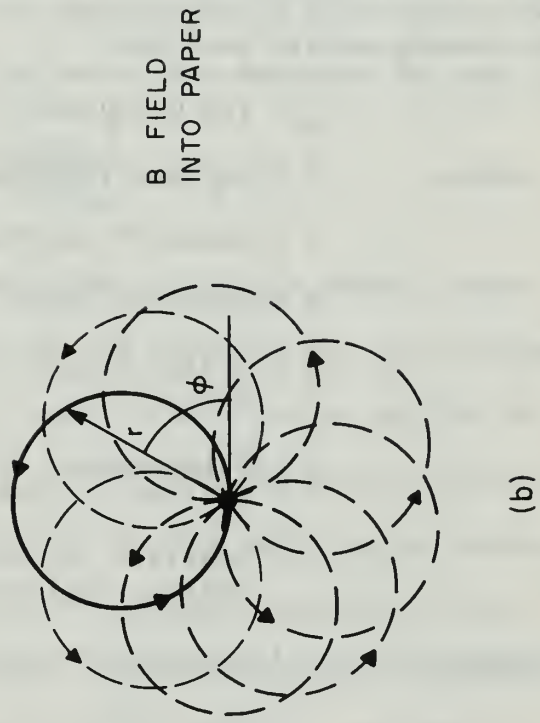
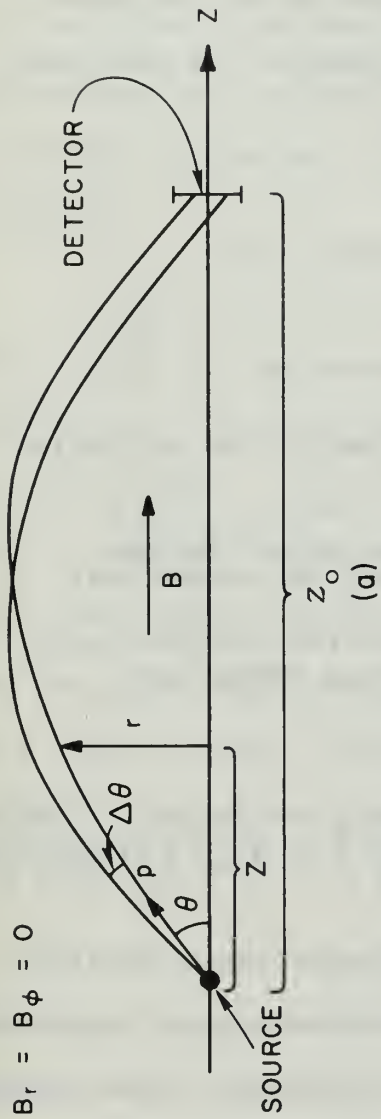


Figure 11. Orbit of Charged Particle in Uniform Magnetic Field

TA-410522-10



Now in order to measure a differential scattering cross section, the solid angle that the finite size detector "sees" must be known. For the axially symmetric case this is  $d\Omega = 2\pi \sin \theta d\theta$ . To evaluate  $d\theta$  consider the various parameters affecting  $Z_o$ , the axis intercept distance. A functional relationship exists such that:

$$Z_o = f(E, \theta, B, \rho, \eta, C)$$

where

$E$  = energy of incident ion

$\theta$  = angle of scatter

$B$  = magnetic field

$\rho$  = radial target displacement from the system axis

$\eta$  = displacement of target atom from the scattering center along the system axis

$C$  = constant for each reaction including mass ratios, inelastic energy losses, etc.

Differentiating this expression gives

$$\Delta Z_o = \left( \frac{\partial Z_o}{\partial E} \right) \Delta E + \left( \frac{\partial Z_o}{\partial \theta} \right) \Delta \theta + \left( \frac{\partial Z_o}{\partial B} \right) \Delta B + \left( \frac{\partial Z_o}{\partial \rho} \right) \Delta \rho + \left( \frac{\partial Z_o}{\partial \eta} \right) \Delta \eta + \left( \frac{\partial Z_o}{\partial C} \right) \Delta C$$

For a specific measurement  $\Delta B$  and  $\Delta C$  are zero. Since analytic expressions for the various derivatives are not known, they must be evaluated numerically by varying  $E$ ,  $\theta$ ,  $\rho$ , and  $\eta$ . Bush, Cook, Heinz, and Rodeback [8] estimate that  $\Delta \rho$  and  $\Delta \eta$  which are due to the finite volume of the scattering region affect  $\Delta \theta$  by no more than 10%. Approximating  $\Delta \rho$  and  $\Delta \eta$  as zero the above expression can be rearranged to  $\Delta \theta = \left( \frac{\partial \theta}{\partial Z_o} \right) \left[ \Delta Z_o - \left( \frac{\partial Z_o}{\partial E} \right) \Delta E \right]$ .

The effect of a small (2%) energy spread was studied and it was concluded that the "effective"  $\Delta\theta$  was not changed. The angular resolution of the apparatus was degraded somewhat in that not all particles scattered within  $\Delta\theta$  of  $\theta$  were collected but this was compensated by the fact that some particles scattered outside of  $\Delta\theta$  were collected. The solid angle can therefore be approximated as

$$d\Omega \simeq 2\pi \sin \theta \left| \left( \frac{\partial \theta}{\partial Z_0} \right) \right| \Delta Z_0$$

where  $\pm \frac{\Delta Z_0}{2}$  is the maximum deviation of the trajectory intercept from  $Z_0$  that will still allow the particle to be collected by the detector.  $\Delta Z_0$  can be calculated by considering the detector geometry and the angle  $\theta_0$  with which the particle intercepts the Z-axis. As an example of how the approximate expression for the solid angle is applied if an analytic expression for  $Z_0 = f(\theta)$  is known, consider again the uniform axially symmetric magnetic field. Recalling that  $Z_0 = \frac{2\pi}{qB} \cos \theta$ , it follows that  $d\Omega \simeq \frac{qB}{p} \Delta Z_0$ .

For the non-uniform axially symmetric field, the procedure for computing trajectories and solid angles was essentially the same as for the uniform case except that the calculations were done numerically on an IBM 360-67 digital computer. The program that accomplished this is explained in Appendix A. A very brief outline of the program is as follows.

- (1) Express the magnetic field along the axis as a 12th order polynomial. This gives  $B_z = (I) \sum_{n=1}^{13} C_n z^{n-1}$  where  $I$  is the magnet current.
- (2) Using this polynomial, a vector potential is found.
- (3) Combining the vector potential with the Lorentz force equation gives a 2nd order non-linear differential equation. This is expressed as two simultaneous, first-order differential equations which are integrated by the DHPGC Subroutine of the Scientific Subroutine Package for the IBM 360-67 computer. The trajectory,  $z_o$ , and  $\theta_o$  are now known.
- (4) The above procedure is done over a selected range of scattering angles and a polynomial expressing  $\theta = f(z_o)$  is generated.
- (5) From  $\theta_o$  and the detector geometry,  $\Delta z_o$  is calculated.
- (6) The solid angle can now be calculated as  $d\Omega(\theta) = 2\pi \left(\frac{290}{360}\right) \sin \theta \left(\frac{\partial \theta}{\partial z_o}\right) \Delta z_o$ . The factor  $\left(\frac{290}{360}\right)$  is present due to the construction of the scattering cell.

Figure 12 shows a series of trajectories computed for  $H^+$  ions with incident energy of 100 eV elastically scattered by Argon.

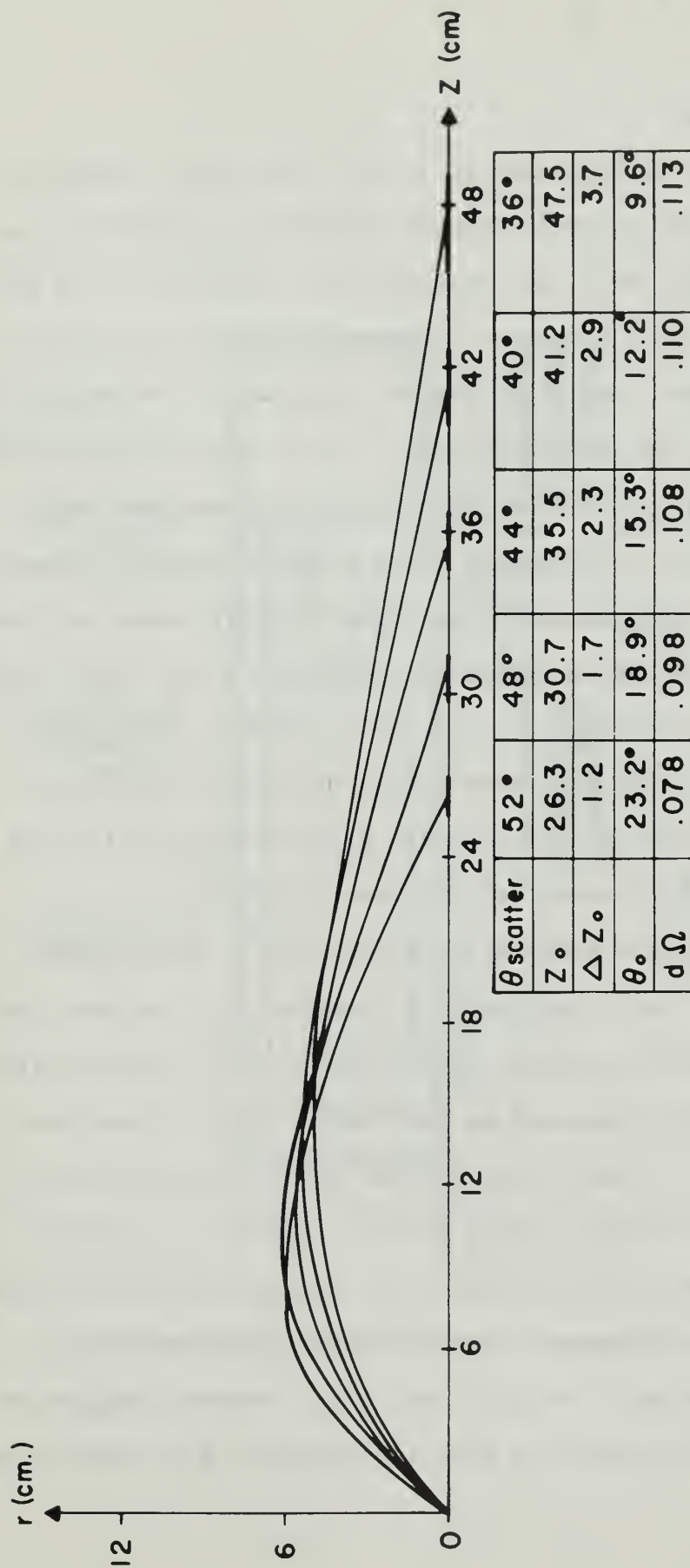


Figure 12. Trajectories of  $H^+$  ions, with 100 eV. Incident energy scattered by argon, in focusing magnetic field with  $I = 4.8$  amps.

#### F. THE DETECTOR.

The detector system employed in this experiment consisted of a Bendix Model 306 Magnetic Electron Multiplier (MEM) which was fed into a Keithly Model 640 Electrometer. Figures 13, 14 and 15 show the detector geometry, a schematic of operation, and a circuit diagram. The principle of operation of the multiplier was as follows. An incident ion was accelerated to about 1500 eV and ejected an electron from the tungsten cathode upon impact. A crossed electric and magnetic field (alnico permanent magnets) imparted a cyclical trajectory to the electron(s) down the dynode strip. The glass dynode and field strips had a high resistance coating of tin oxide and antimony that sustained the electric field. Each time the electrons struck the dynode strip multiplications occurred so that when the electrons were collected by the anode, a gain of about  $10^4$  had been realized.

Unfortunately the MEM had to be operated in the focusing magnetic field. This resulted in a sideways drift of the electrons moving down the dynode strip so that all of the electrons generated were not collected at the anode. This in fact made the MEM gain a very sensitive function of its position in the focusing magnetic field. The procedure used was to calibrate the MEM under the same environment that existed during the actual cross section measurements. Specifically, this consisted of:

- (1) measuring the gain using  $H_2^+$  ions with a focusing magnet current of 6.6 amperes with the detector position,  $Z_0$ , varied from



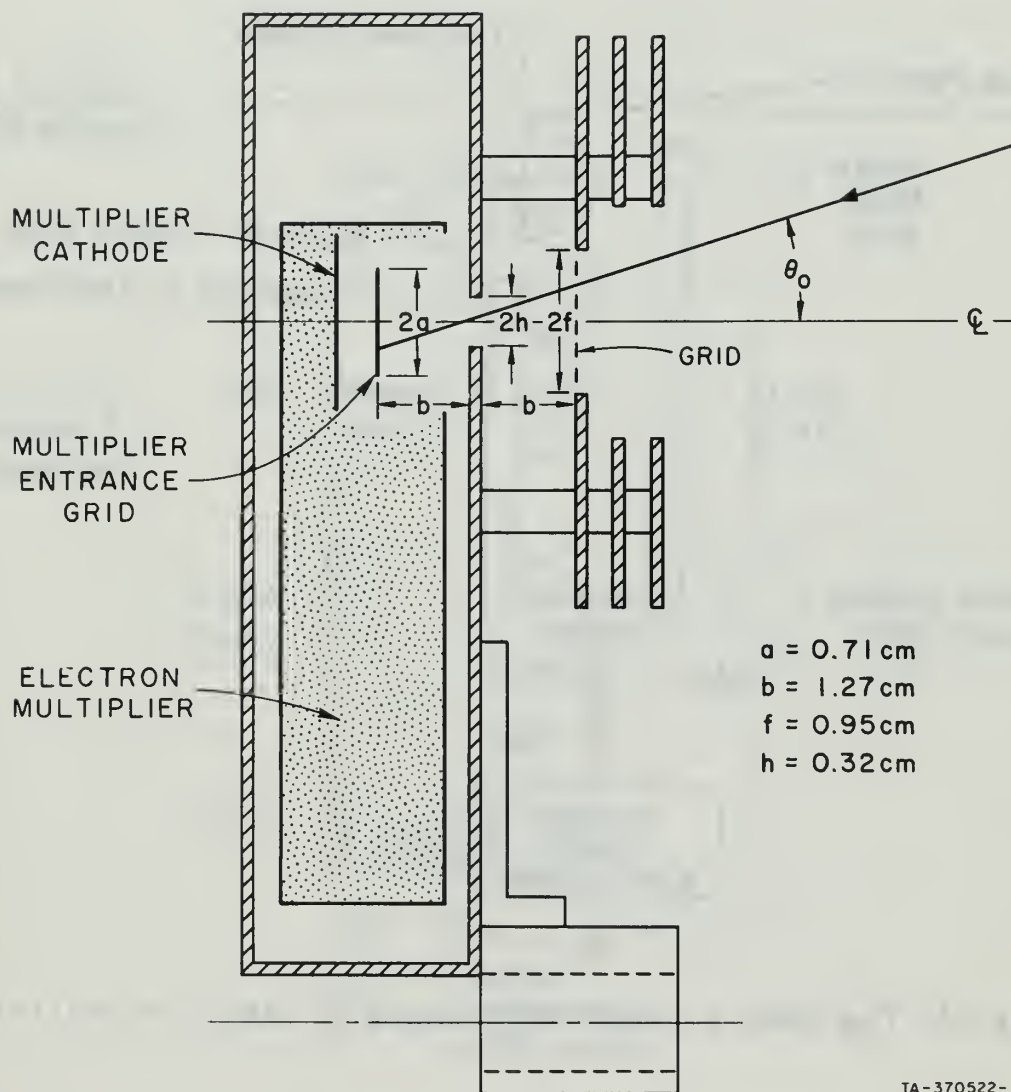


Figure 13. Detector Aperture Geometry.



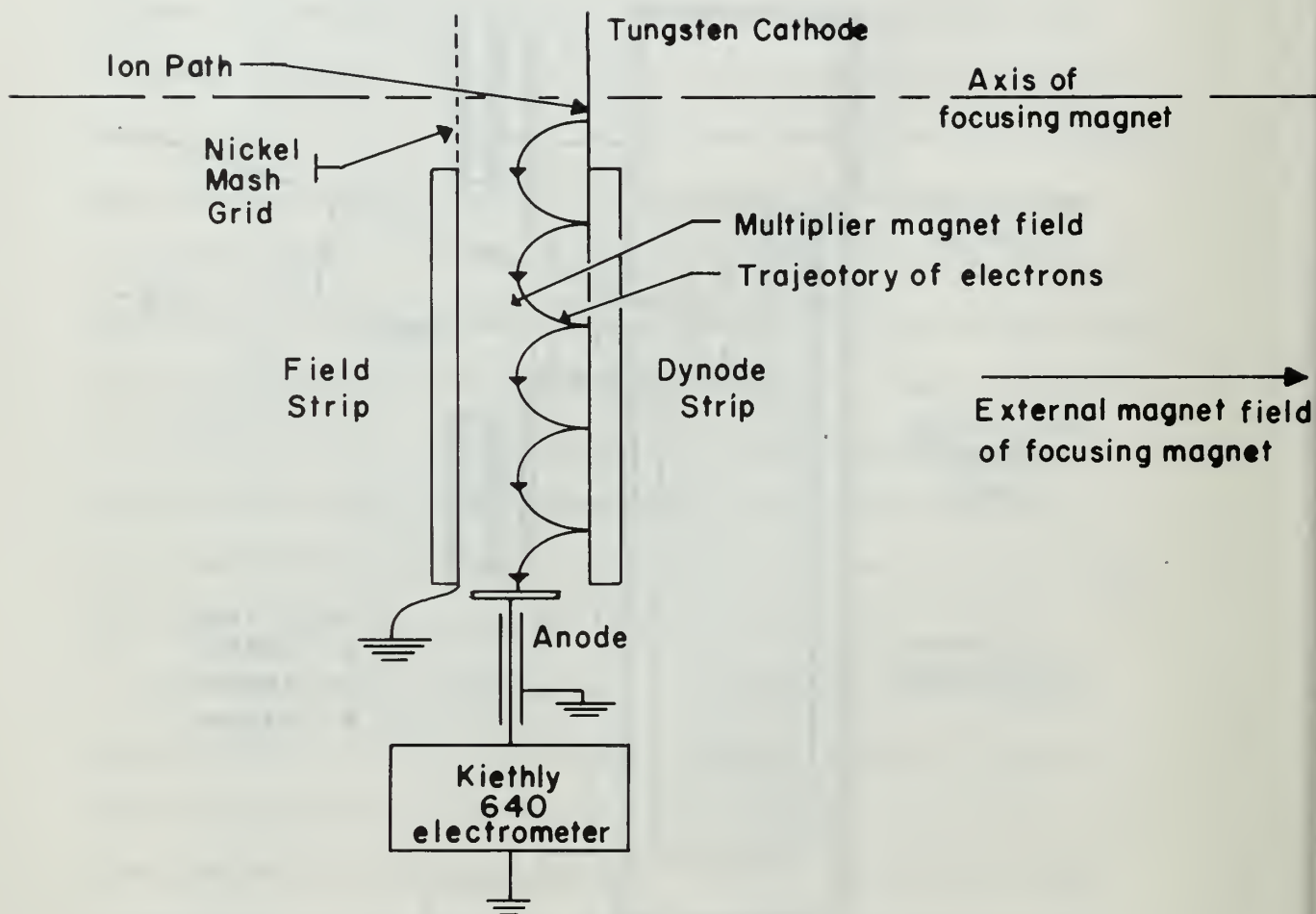
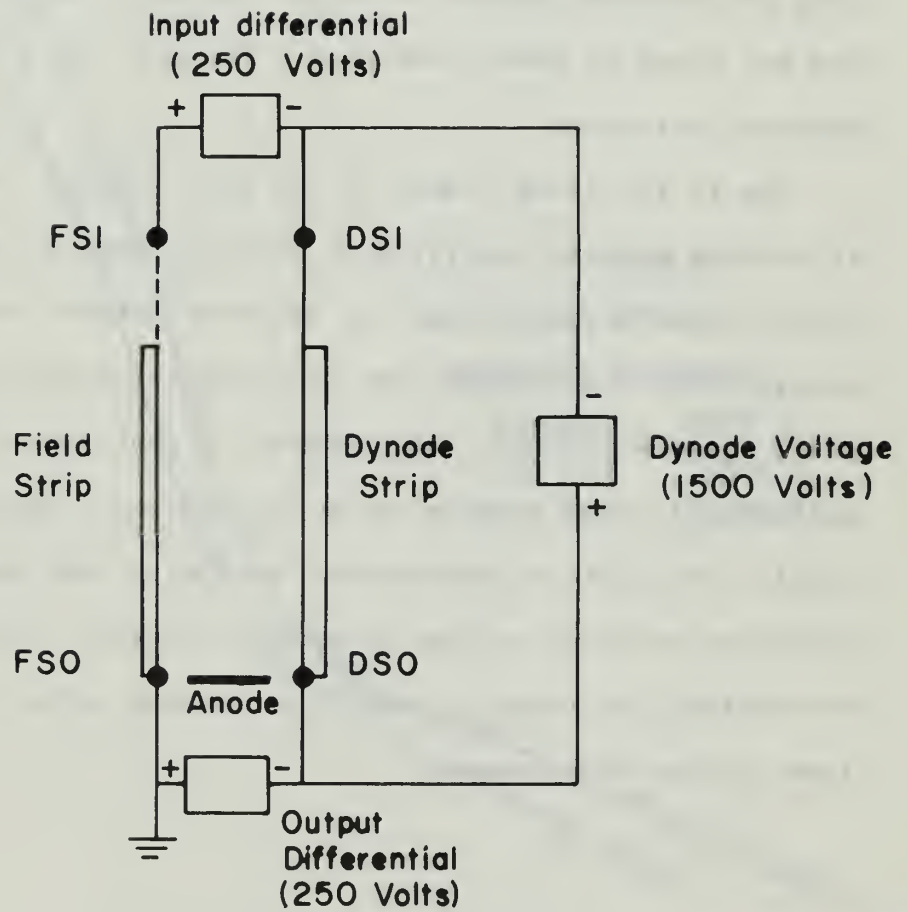


Figure 14. The bendix model 306 magnetic electron multiplier



**Figure 15.** Circuit Diagram for Electron Multiplier.

30.5 to 47.5 centimeters from the scattering cell, (2) measuring the gain using  $H^+$  ions with a focusing magnet current of 4.8 amperes with the detector position,  $Z_0$ , varied from 28.5 to 42.5 centimeters from the scattering cell. Since the focusing magnetic field was a known function of current and position, the two gains are plotted against magnetic field in Fig. 16. The gain for  $H_2^+$  ions was measured before and after the cross section measurements and was found to remain constant. The gain for  $H^+$  ions was measured only once.

Due to the steep slopes of the gain curves, a small error in setting detector position or focusing magnet current will result in a large error in the detector current reading. This, coupled with the tedious task of calibrating the detector for every species, energy, and magnetic current that a cross section measurement is to be made, made this detector system less than ideal. For further experimental work with this apparatus, a different detector system is being considered. This may consist of counting the output pulses from the MEM rather than integrating them with an electrometer.

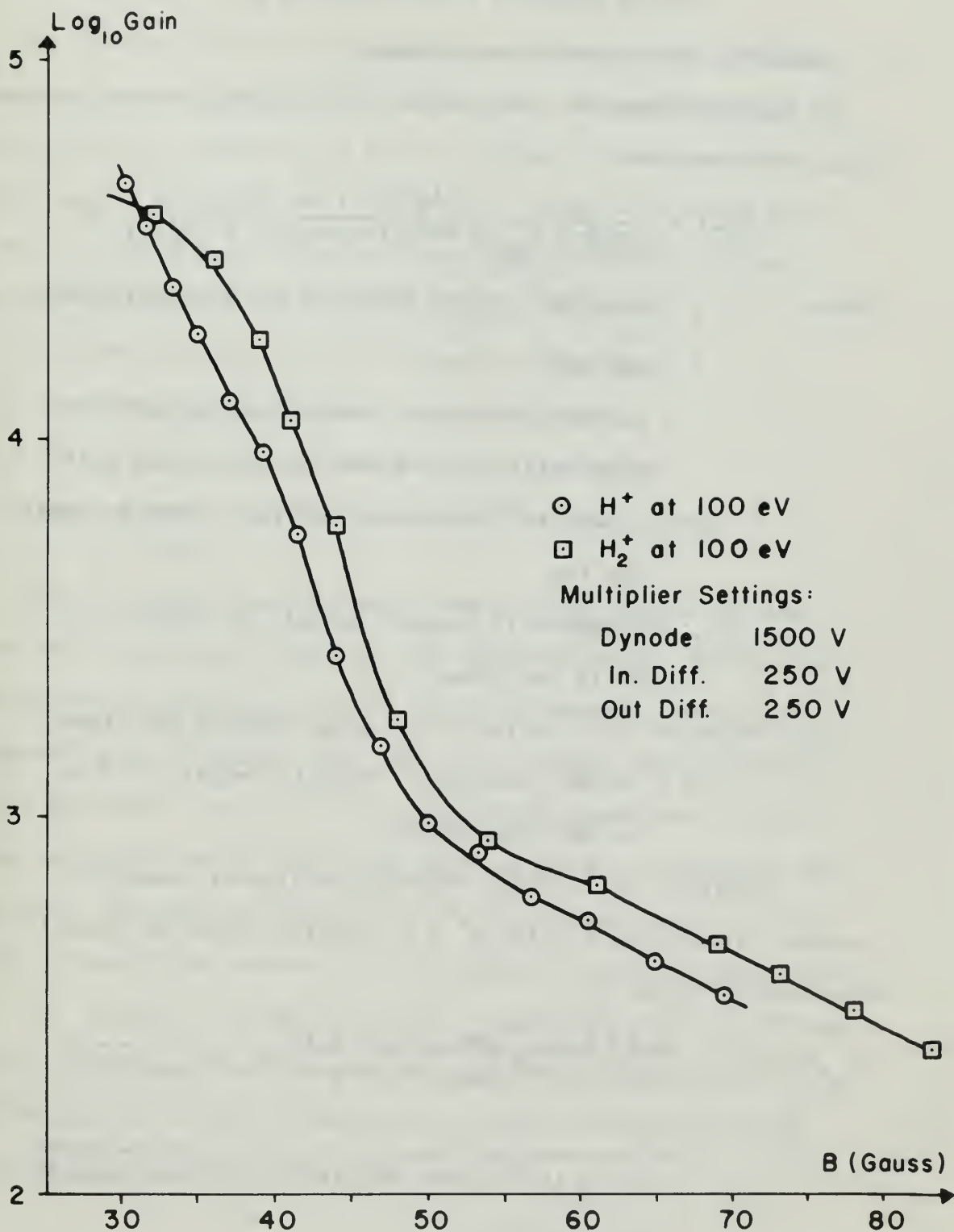


Figure 16. Multiplier gain vs. magnetic field.

#### IV. EXPERIMENTAL RESULTS

##### A. LABORATORY CROSS SECTION MEASUREMENT.

The equation used for calculating a differential cross section in the laboratory was

$$d\sigma(\theta) = \frac{I_D/G}{I_i \times (\rho \times P_{sc} \times \text{Corr. Factor}) \times t \times d\Omega(\theta)} \text{ cm}^2.$$

where  $I_D$  = detector current measured by an electrometer

$G$  = MEM gain

$I_i$  = Incident ion beam. Sum of the currents to Beam Collector and Rear of Scattering cell.

$\rho = 3.54 \times 10^{16}$  particles/cm<sup>3</sup>-torr based on ideal gas law.

$P_{sc}$  = Pressure in scattering cell as measured by VG-1A ion gauge

Corr. Factor = .617; corrects ion gauge reading for Argon

$t$  = target thickness. Normally equal to .3 cm in this experiment

$d\Omega(\theta)$  = Solid angle computed by digital computer.

A sample calculation for the  $H^+ + Ar$  reaction showing typical experimental values is

$$\begin{aligned} \sigma_{H^+}(41.9^\circ) &= \frac{(1.85 \times 10^{-9} \text{ amp.})/1.27 \times 10^4}{(1.41 \times 10^{-8} \text{ amp.})(3.54 \times 10^{16} \text{ cm}^{-3}\text{-torr}^{-1})} \times \\ &\quad \frac{1}{(1.38 \times 10^{-3} \text{ torr} \times .617)(0.3 \text{ cm})(0.109 \text{ sterad})} \\ &= 1.07 \times 10^{-17} \text{ cm}^2 \end{aligned}$$



B. MEASUREMENT OF THE  $\underline{H}^+ + \text{Ar} \rightarrow \underline{H}^+ + \text{Ar}$  CROSS SECTION.

The differential scattering cross section for this reaction was measured from  $39.2^\circ$  to  $50^\circ$ . Five runs were made and the data points are displayed in Fig. 17 along with the computed cross section using the Byatt potential. Figure 18 shows the average of the 5 runs along with the computed cross section.

Important parameters for the measurements included:

- (1) Incident energy of  $H^+$  ions equal to 100 eV.
- (2) Focusing magnet current equal to 4.8 amps.
- (3) Solid angle typically equal to 0.1 steradians.
- (4) Argon pressure in scattering cell typically equal to  $1 \times 10^{-3}$  torr.

Figure 18 shows that the experimental curve, while having about the same overall slope as the computed curves, differs in magnitude by a factor of about 6. This difference, while not catastrophic, was greater than expected. First, there may have been a systematic error in the experimental apparatus. A possible systematic error could have been an error in measuring the MEM gain. The gain was measured with an incident beam several orders of magnitude greater than the beam of scattered particles. Thus, if the MEM gain were a (slowly) increasing function of input current, the measured gain would be greater than the gain for the smaller beam of scattered particles. This would result in the measured cross sections being too small.

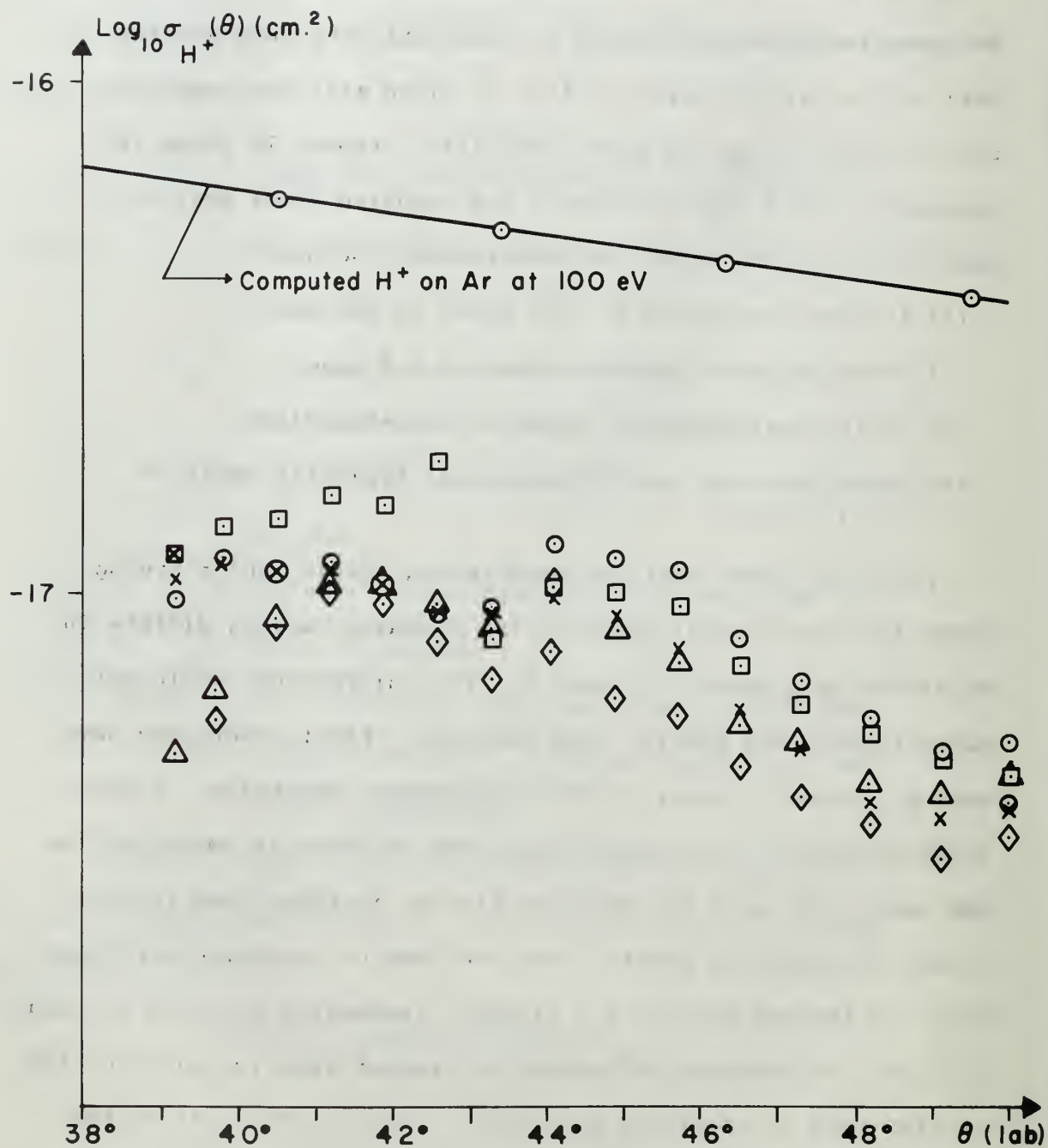


Figure 17. Experimental measurements of  $\text{H}^+ + \text{Ar} \rightarrow \text{H}^+ + \text{Ar}$  at 100 eV.

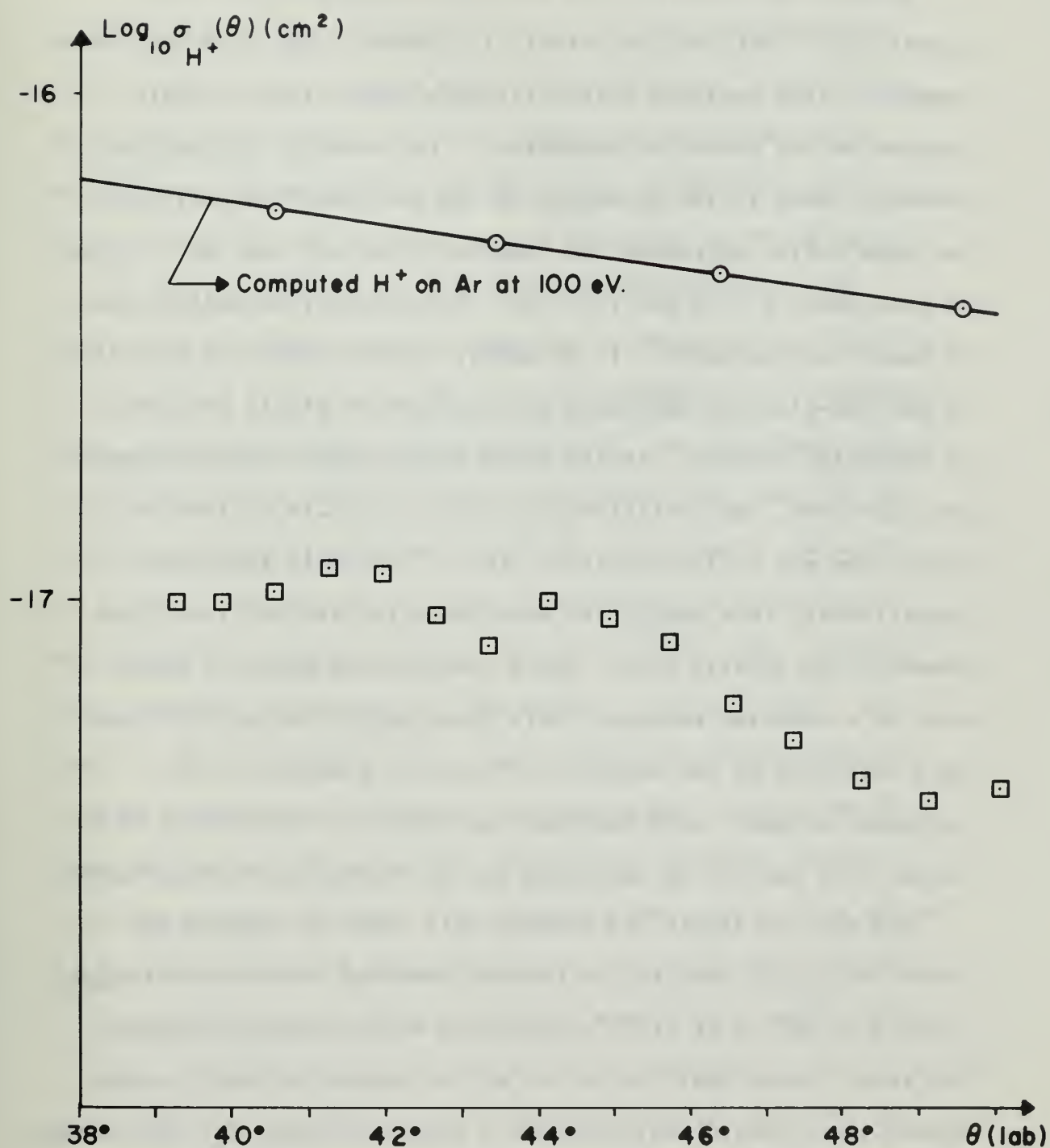


Figure 18. Average of experimental measurements of  $H^+ + \text{Ar} \rightarrow H^+ + \text{Ar}$  at 100 eV.

Second, the potential may have been inadequate for this application. Varying the potential parameters revealed that the computed cross sections were relatively insensitive to small changes in the potential parameters. For example, varying the dominate terms in the potential by 30% such that the collision was made softer decreased the computed cross sections by a factor of only about 2. It was felt that the potential parameters were at least this accurate. It is noted, however, that the potential is Hartree-like and therefore will reflect no atomic structure or inelastic process. At the large angles where this experiment was conducted, the collisions are relatively hard so that the Argon atom may well be excited. The  $H^+$  ion would then have significantly less energy and momentum after the collision compared to the elastic case. Since the focusing magnetic field acts as a momentum analyzer, only elastically scattered  $H^+$  ions were collected by the detector. Thus, the presence of an inelastic process could decrease the elastic cross section by a factor of 6 and not be accounted for in the Hartree-like potential.

The work of Aberth and Lorents [11] tends to support the second analysis. Aberth and Lorents measured the scattered signal profile of  $He^+$  on Ar at  $10^\circ$  and 400 eV with an energy analyzer. The result shows that for  $He^+$  on Ar, an inelastic event is more likely than elastic scattering by a factor of about  $2\frac{1}{2}$ . The energy lost by  $He^+$  in inelastic events was on the order of 10 to 15 eV.

Applying this to the case of  $H^+$  on Ar, it seems reasonable to expect protons to be a more efficient projectile for exciting Ar than  $He^+$  and therefore could account for the factor of 6. Furthermore, inelastically scatter protons with energy after collision of 85 - 90 eV would not be collected by the detector.

The choice between the computed and experimental cross sections was accomplished by comparing the data in Fig. 18 with data supplied by Magnuson, Carlston, and Snyder [9]. Magnuson et al also measured the cross section of  $H^+$  on Ar although their measurements were made for scattering angles less than  $20^\circ$  and energies ranging from 150 eV to 800 eV. Meaningful comparison of the data was possible by using a reduced plot outlined by Smith, Marchi, Aberth, Lorents, and Heinz [10]. This reduced plot consists of plotting  $\tau = E\theta$  versus  $\rho = \theta \sin \theta \sigma(\theta)$ . By the use of this scaling law, cross section curves obtained at various energies are reduced to a single line. The reason is that the product  $E\theta$  represents essentially the same encounter with the atomic potential. By comparing the data in this manner it was found that the two experimental curves agreed to within a few percent and the unaveraged data in fact overlapped. Thus, it was concluded that the experimentally determined cross sections were probably correct. It is further noted that the data of Magnuson, et.al. covered a much larger range of  $\tau = E\theta$  than this experiment and does reflect atomic structure such as discussed in the preceeding two paragraphs.



C. MEASUREMENT OF THE  $\text{H}_2^+ + \text{Ar} \rightarrow \text{H}_2^+ + \text{Ar}$  CROSS SECTION.

The differential scattering cross section for this reaction was measured from  $38.8^\circ$  to  $49.7^\circ$ . Five runs were made and the data points are displayed in Fig. 19. The average of the 5 runs is displayed in Fig. 20. Important parameters for this measurement included:

- (1) Incident energy of  $\text{H}_2^+$  ion beam equal to 100 eV.
- (2) Focusing magnet current equal to 6.6 amperes.
- (3) Solid Angle typically equal to 0.1 steradians.
- (4) Argon pressure in the scattering cell typically equal to  $1 \times 10^{-3}$  torr.

From Fig. 20 it is seen that the overall slope of the experimental curve is essentially flat. That the cross section does not decrease significantly with increasing angle is possibly due to the following instrumental effect. Some particles scattered outside of the computed solid angle may reach the detector through multiple collisions with the walls of the apparatus and still have sufficient energy to overcome the detector grid bias. The signal due to these extraneous particles could not be subtracted out in that they essentially behaved like the "real" particles scattered into  $d\Omega$ . That is, the signal due to extraneous particles was proportional to the incident  $\text{H}_2^+$  beam intensity and to the pressure in the scattering cell. Normally, this extraneous signal is negligible compared to the signal from particles scattered within  $d\Omega$ . However, in this case at the larger angles the

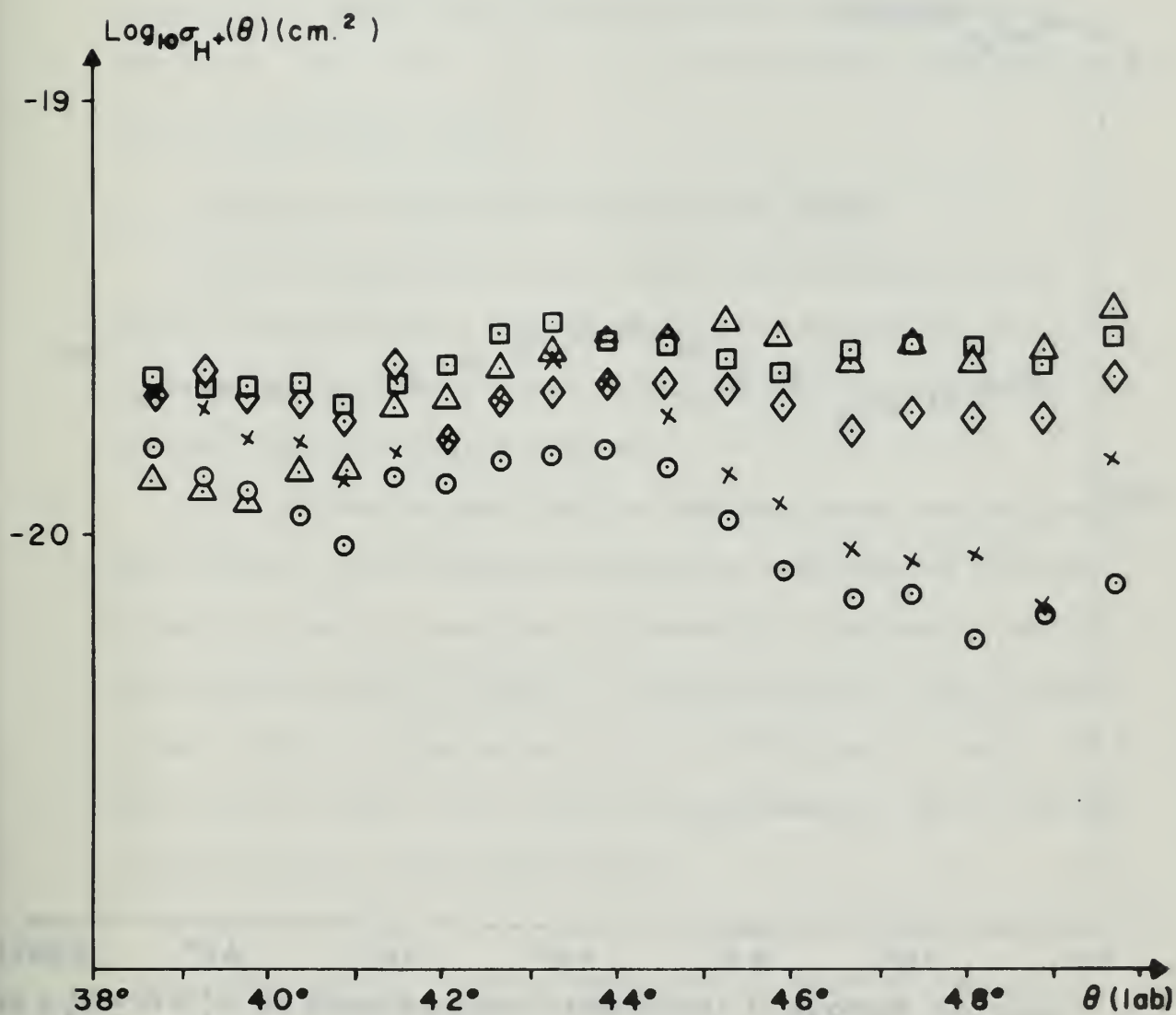


Figure 19. Experimental measurements of  $\underline{H_2^+} + \text{Ar} \rightarrow \underline{H_2^+} + \text{Ar}$  at 100 eV.

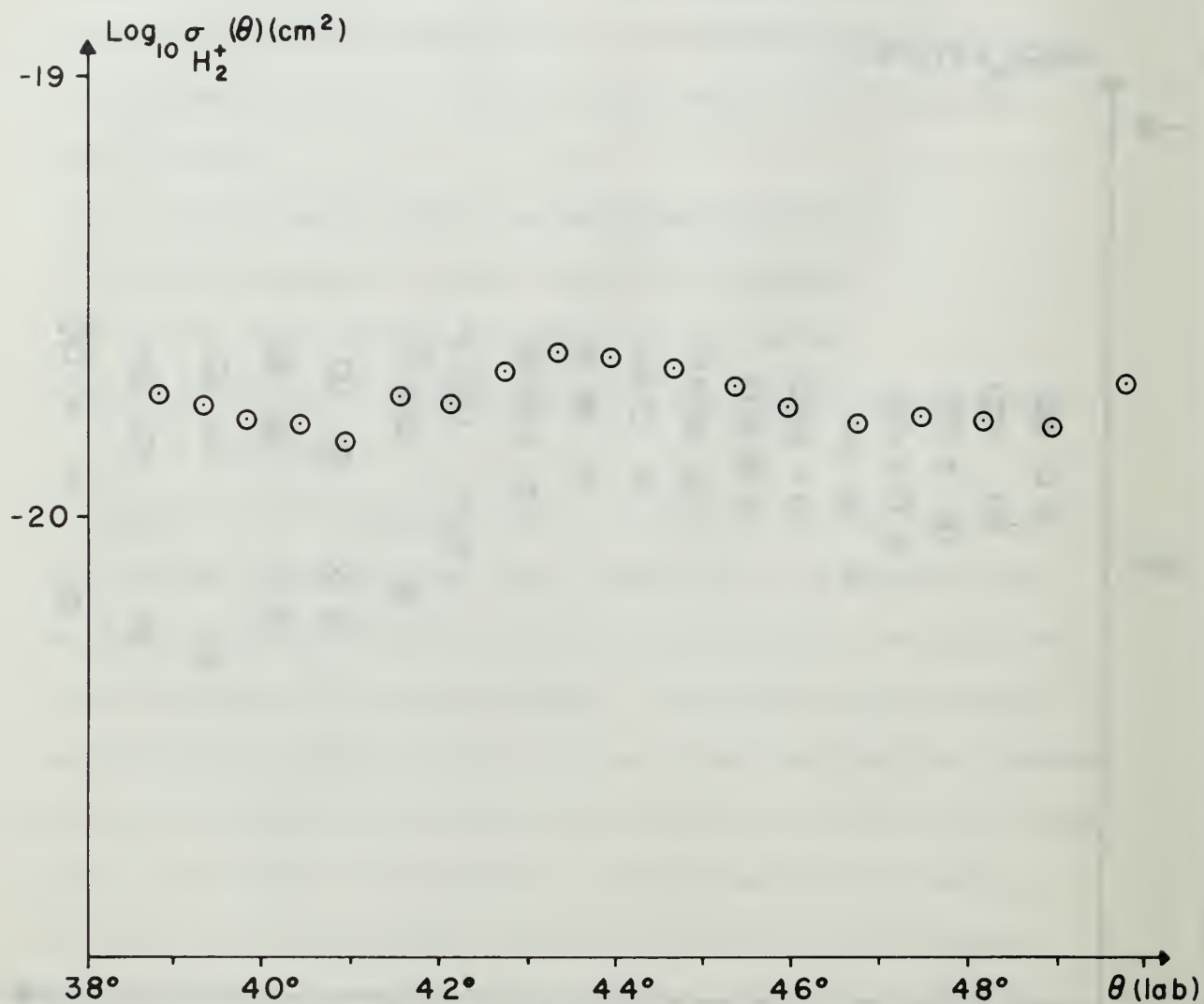


Figure 20. Average of experimental measurements of  $\text{H}_2^+ + \text{Ar} \rightarrow \text{H}_2^+ + \text{Ar}$  at 100 eV.

detector signal was quite small, typically on the order of  $0.3 \times 10^{-12}$  amperes. Therefore, perhaps up to 50 percent of the measured signal could have been due to these extraneous particles. This would also account for the wider dispersion of data at the larger angles.

#### D. EXPERIMENTAL RESULTS AND THE CLASSICAL MODEL.

Since it could not be ascertained with certainty as to whether the computed or experimental cross section for  $H^+$  on Argon was more accurate, the analysis of the classical model was done from both points of view.

First, it was assumed that the computed cross section for  $H^+$  was correct. The difference between the experimental and computed cross section was then attributed to a systematic error and the experimental  $H^+$  data was normalized to fit the computed curves. This was done by moving the  $H^+$  data up by a factor of 6. Now the  $H_2^+$  on Argon cross section measurement had the following similarities with the  $H^+$  measurement:

- (1) Approximately the same focusing magnetic field (see Fig. 16).
- (2) Approximately the same excursion in detector position.
- (3) Approximately the same calculated solid angle.
- (4) The gain curves for both measurements have about the same shape (see Fig. 16).

It was therefore concluded that if a systematic error were present, it should have affected the  $H_2^+$  measurement by about the

same magnitude. Therefore, the  $H_2^+$  data was also increased by a factor of 6. The results of this normalization are shown in Fig. 21. It is seen that the  $H_2^+$  on Argon experimental data presented in this manner lies below the predicted curve by a factor of about 14.

Second, it was assumed that the experimentally measured  $H^+$  on Argon cross section was more accurate than the computed. Since the classical model predicts that the cross section for  $H_2^+$  is proportional to the square of the  $H^+$  cross section (Eq. 8), the predicted curve for  $H_2^+$  on Argon in Fig. 21 would be moved down by a factor of  $(6)^2$  or 36. Figure 22 illustrates this. In this case, it is seen that the experimental measurement for  $H_2^+$  on Argon lies below the cross section predicted by the classical model by a factor of about 2 to 3.



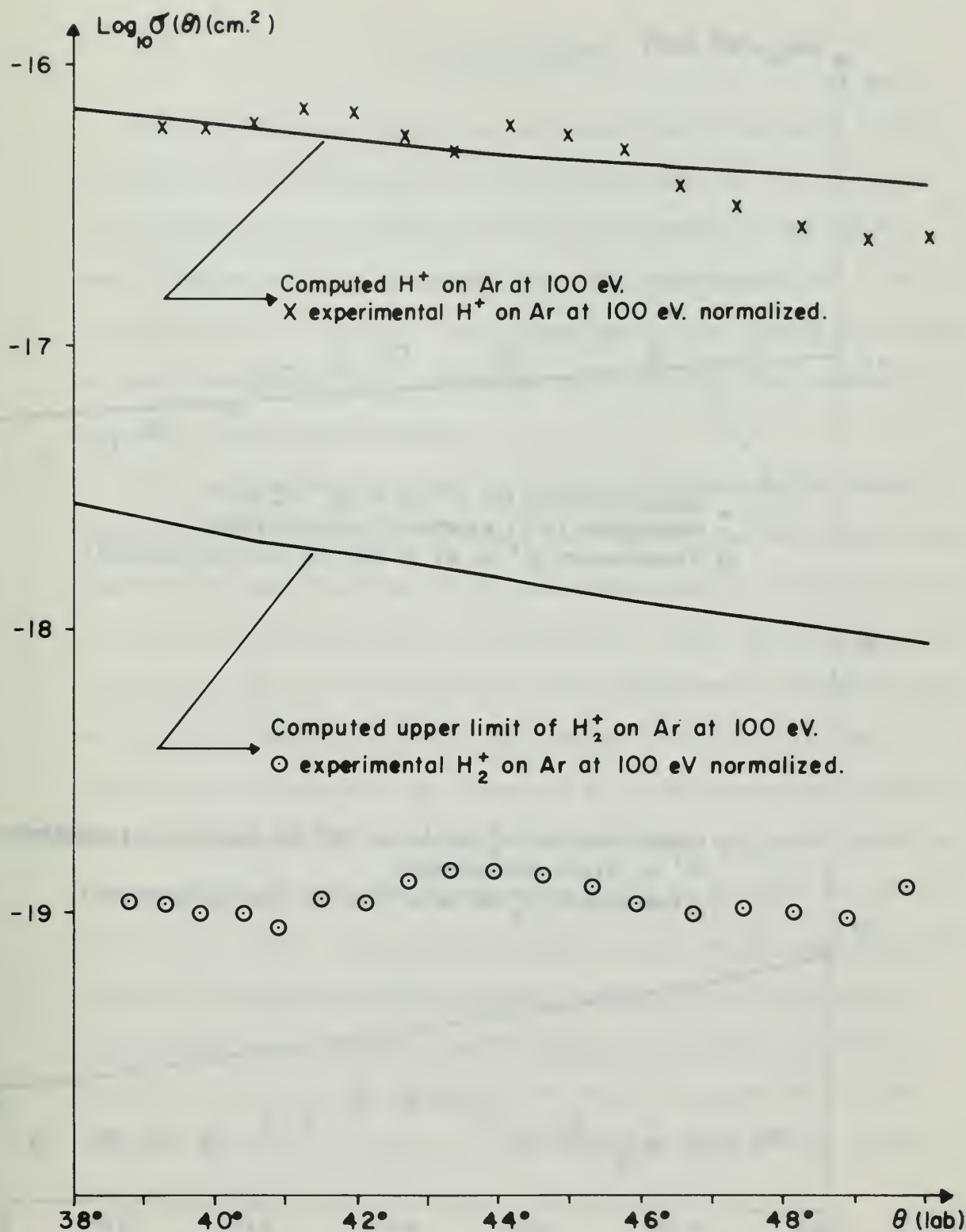


Figure 21. Analysis of experimental measurement assuming a systematic error.

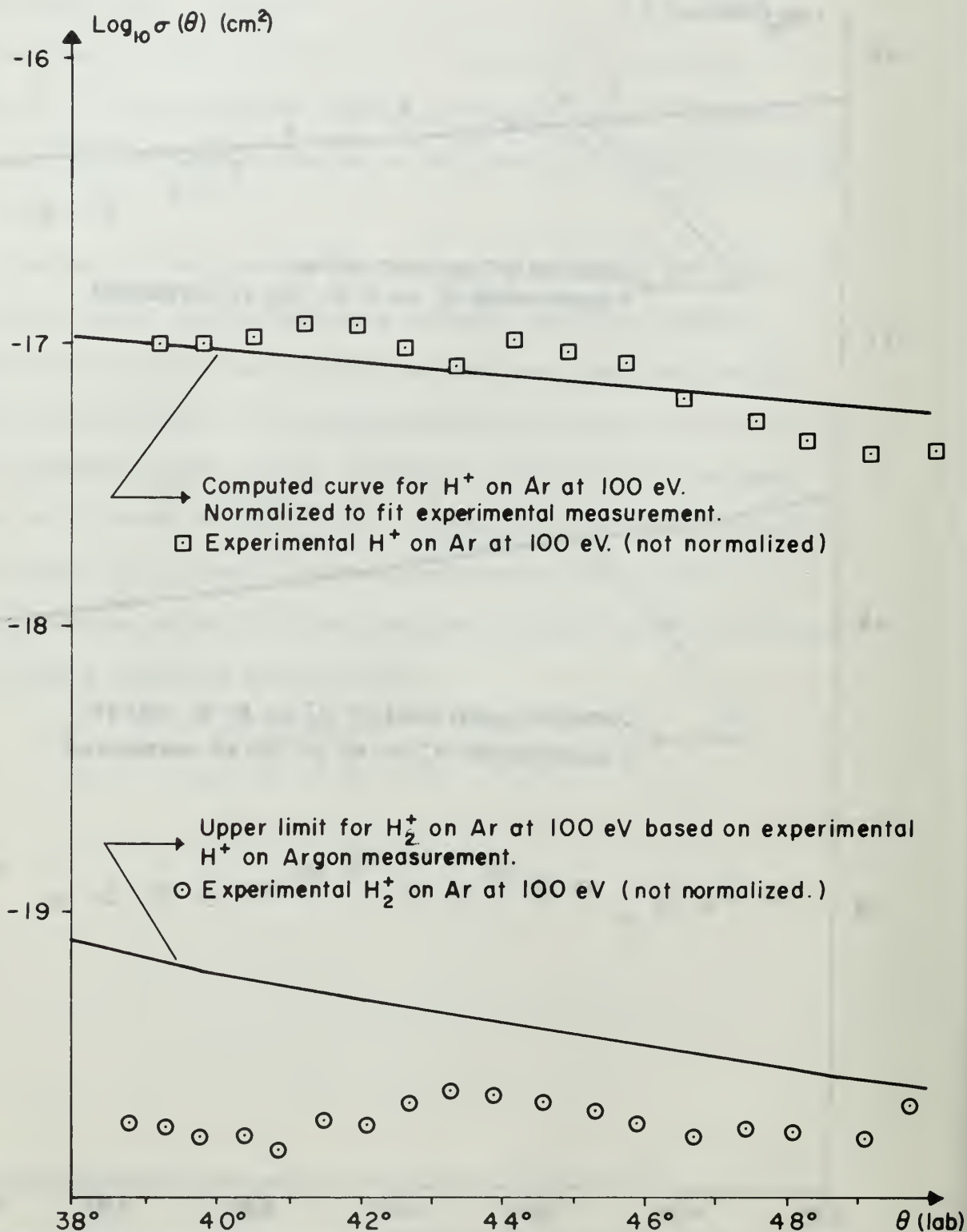


Figure 22. Analysis of experimental measurement assuming no systematic error.

## V. CONCLUSIONS

The experimental results given above can be analyzed in two distinct ways: (1) Assume that the theoretical  $H^+ + Ar$  curve is correct and that a systematic error was present in the experimental measurements. (2) Assume that the experimental  $H^+ + Ar$  cross section is correct. We present below the conclusions based on both assumptions and our reason for believing that method (2) is more likely to be correct.

If a systematic error were present and affected the measurements of both the  $H^+$  and  $H_2^+$  cross sections by the same magnitude, then it was seen that the classical model predicts a cross section for  $H_2^+$  too large by a factor of about 14. That the actual cross section for  $H_2^+$  is so much smaller than predicted is probably due to the two effects previously discussed. That is: (1) the orientation probability was computed by considering the maximum area enclosed by the  $\Delta\theta = g(\Delta b)$  curve and (2) the model neglected the possibility that the  $H_2^+$  molecule might be excited during the collision process. That the predicted cross section was so much greater than observed would perhaps make the classical model useful only for predicting upper limits of  $H_2^+$  cross sections. However in view of the agreement of our  $H^+$  on Argon data with Magnuson et.al. [9], this is considered the less likely of the two conclusions.

If both experimental measurements are correct, then it is seen that the classical model predicts an  $H_2^+$  cross section too large

by a factor of about 2 to 3. This would make the classical model useful for predicting  $H_2^+$  cross sections on an absolute basis.

This is considered to be the more likely of the two conclusions.

Assuming that the classical model is essentially correct the following simple refinement is proposed: Recalling equation (3) it was seen that the orientation probability could be written as

$$P = \frac{S}{2\pi l^2}$$

where  $S$  was the area enclosed by the  $\Delta\theta = g(\Delta b)$  curve. Since  $S$  could not be determined exactly, an upper limit was obtained by considering the maximum values for  $\Delta\theta$  and  $\Delta b$  respectively when the other variable was zero. This in fact gave four points on the  $\Delta\theta = g(\Delta b)$  curve, namely:

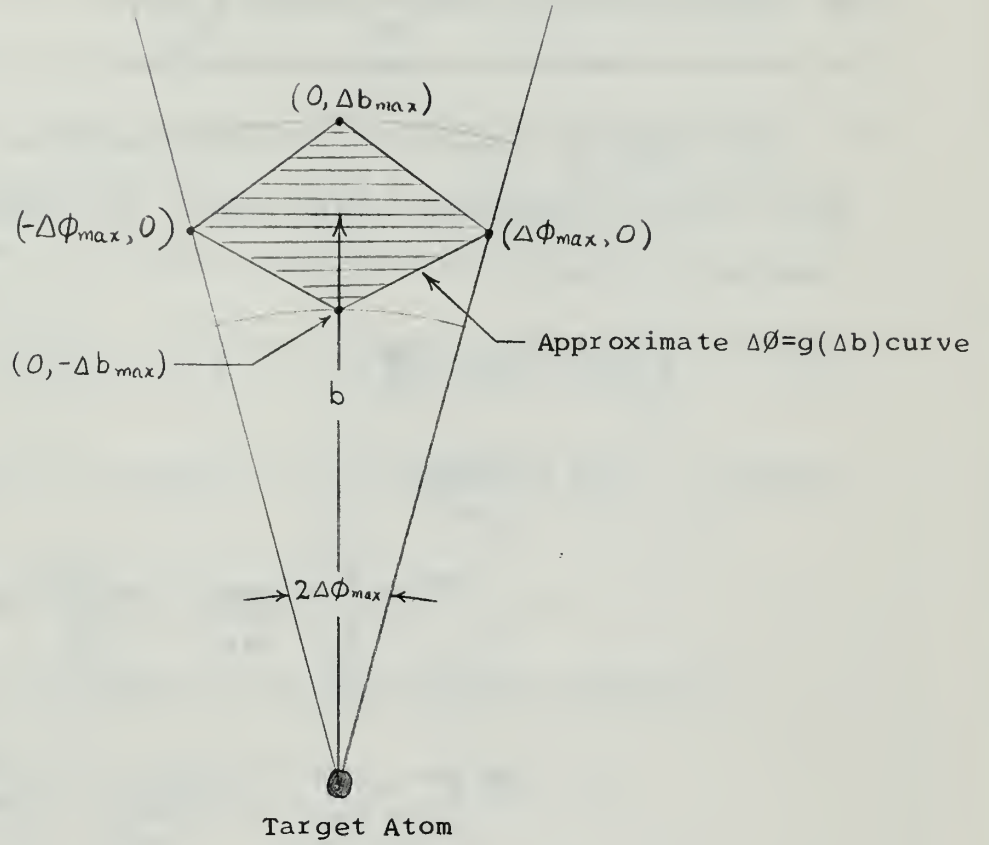
$$\Delta\theta = 0, \Delta b = + \Delta b_{\max}$$

$$\Delta\theta = 0, \Delta b = - \Delta b_{\max}$$

$$\Delta b = 0, \Delta\theta = + \Delta\theta_{\max}$$

$$\Delta b = 0, \Delta\theta = - \Delta\theta_{\max}$$

A first approximation to the  $\Delta\theta = g(\Delta b)$  curve can therefore be obtained by simply connecting these points with straight lines. The following sketch illustrates this.



The area enclosed by this first approximation is

$$S = \frac{1}{2} [2(\Delta b_{\max}) \Delta \theta = 0] [2b(\Delta \theta_{\max}) \Delta b = 0] = \frac{1}{2} S_{\max}$$

which leads to  $P \approx \frac{1}{2} P_{\max}$

$$\text{and } \sigma_{H_2^+}(\theta) \approx \frac{4D}{\pi l^2 E_0} [\sigma_{H^+}(\theta)]^2. \quad (9)$$

Equation (9) predicts the experimentally observed cross section for  $H_2^+$  to within the accuracy of the experiment.



## APPENDIX A

1. Computer Program for  $\sigma_{H^+}(\theta)$  and  $\sigma_{H_2^+}(\theta)$ .
- 

This computer program solves the following set of equations for classical differential scattering in the center of mass coordinate system.

$$\sigma_{H^+}(\theta) = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$$

where  $\theta = \pi - 2bU$

$$U = \int_{r_0}^{\infty} \frac{1}{r^2} \left[ 1 - \frac{V(r)}{\frac{1}{2}\mu V_0^2} - \frac{b^2}{r^2} \right]^{-\frac{1}{2}} dr$$

$$r_0 = \text{largest positive root of } 1 - \frac{V(r)}{\frac{1}{2}\mu V_0^2} - \frac{b^2}{r^2} = 0$$

with  $\mu$  = reduced mass of the system

$V_0$  = velocity of incident particle in the laboratory system

$V(r)$  = scattering potential

In this case the scattering potential as given by Byatt [3] for Argon converted to electron volts is  $V(R) = \frac{1}{R}(Ae^{\alpha R} + Be^{\beta R} + Ce^{\gamma R})$  with  $R$  in units of Bohr radii ( $0.5292\text{\AA}$ ) where

$$A = 411.4 \quad \alpha = -1.676$$

$$B = -117.5 \quad \beta = -3.127$$

$$C = 195.9 \quad \gamma = -9.625$$

An outline of this program is as follows:

1. Read in the desired incident energies, mass of proton, mass of target atom, disassociation energy, and potential parameters.

2. Select an impact parameter,  $b$ . From an initial value,  $b$  is increased in units of  $.05 a_0$  where  $a_0$  is the first Bohr radius.

3. Solve for the largest positive root of

$$1 - \frac{V(r_0)}{\mu V_0^2/2} - \frac{b^2}{r_0^2} = 0 \text{ using the Newton-Raphson method.}$$

4. Evaluate the integral,  $U = \int_{r_0}^{\infty} \left[ 1 - \frac{V(r)}{\frac{1}{2}\mu V_0^2} - \frac{b^2}{r^2} \right]^{-\frac{1}{2}} \frac{1}{r^2} dr$

using the Gauss-Mahler quadrature formula

$$U = \frac{\pi}{r_0} \left[ \left( \cos \frac{5\pi}{12} \right) g(x_1) + \left( \cos \frac{3\pi}{12} \right) g(x_2) + \left( \cos \frac{\pi}{12} \right) g(x_3) \right]$$

where  $g(x_i) = \left[ 1 - \frac{V(r_0/x_i)}{\frac{1}{2}\mu V_0^2} - \frac{b^2}{(r_0/x_i)^2} \right]^{-\frac{1}{2}}$

with  $x_1 = \cos \frac{\pi}{12}$ ,  $x_2 = \cos \frac{3\pi}{12}$ ,  $x_3 = \cos \frac{5\pi}{12}$ . This procedure was taken from Bates, Cook, and Smith [2].

5. From  $\theta = \pi - 2bU$ , evaluate  $\left| \frac{d\theta}{db} \right| = \left| 2b + 2b \frac{dU}{db} \right|$ .  $\frac{dU}{db}$  is obtained from the analytic expressions

$$U = f(r_0, b) \text{ and } 1 - \frac{V(r_0)}{\mu/2 V_0^2} - \frac{b^2}{r_0^2} = 0 \text{ in a straight-forward}$$

manner using the chain-rule of differentiating  $\frac{dU}{db} = \frac{\partial U}{\partial b} + \frac{\partial U}{\partial r_0} \frac{dr_0}{db}$ .

6. Solve for  $\sigma_{H^+}(\theta) = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$ .

7. Solve for the orientation probability,  $P = \frac{8D}{\pi l^2 E_o} \sigma_{H^+}(\theta)$ .

8. Solve for  $\sigma_{H_2^+}(\theta) = P \sigma_{H^+}(\theta)$ .

9. Write out incident energy,  $b$ ,  $r_o$ ,  $\theta$ ,  $\sigma_{H^+}(\theta)$ ,  $P$ ,  $\sigma_{H_2^+}(\theta)$ .

Computations are done in units of Bohr radii, but  $\sigma_{H_2^+}(\theta)$  and  $\sigma_{H^+}(\theta)$  are converted to  $\text{cm}^2$  at the end of the program. The following is a list of key symbols used in the computer program:

DENER = Disassociation Energy,  $D$ , in units of eV.

RHO(J) = Impact parameter,  $b$ , in units of Bohr radii.

EV(K) = Incident ion energy in units of eV.

$ET = \frac{1}{2} \mu \frac{EV(K)}{M_{H^+}}$  definition

$V = \frac{V(R)}{ET} R$  convenient form of the potential in this program

$DV = \frac{dV}{dR}$

DEG(J) = scattering angle in degrees converted to laboratory system

SIGMA =  $\sigma_{H^+}(\theta)$

CS =  $\sigma_{H_2^+}(\theta)$

```

// EXEC FORTCLG, REGION, GO=160K, TIME, GO=10
// FORT. SYSIN DD *
C THIS PROGRAM SOLVES THE CLASSICAL EQUATIONS FOR DIFFERENTIAL
C SCATTERING
C IMPLICIT REAL*4(A-H,O-Z)
C DIMENSION EV(10), RHO(101), THETA(101), CSL(101), DEG(101), THETA(101)
C DIMENSION RATIO(10)
C READ IN POTENTIAL PARAMETERS, BOHR RADIUS, DISSOCIATION ENERGY,
C INITIAL VALUES
A0=5.29167E-11
A=18.0*1.6021E-19*8.9874E+09*(+.84)/A0
B=18.0*1.6021E-19*8.9874E+09*(-.24)/A0
C=18.0*1.6021E-19*8.9874E+09*(+.40)/A0
ALPHA=1.13*2.620741*(-0.566)
BETA=1.13*2.620741*(-1.056)
GAM=1.13*2.620741*(-3.25)
DENER=2.648
ITN=0
RHO(0)=-0.05
EV(0)=600.0
NO=1
DO 15 K=1,5
C THIS DO-LOOP SOLVES PROBLEM AT DESIRED INCIDENT ENERGIES.
L=K-1
EV(K)=EV(L)-100.
R=200./EV(K)
NO=NO+1
IF(NO-2)19,16,17
16 NOA=1
GO TO 19
17 NOA=2
IF(NO-11)19,18,19
18 NOA=3
19 CONTINUE
DO 6 J=1,101
C THIS DO-LOOP SOLVES PROBLEM AT DESIRED IMPACT PARAMETERS.
N=J-1
THE NEXT 20 STEPS SOLVE FOR 'R', THE DISTANCE OF CLOSEST APPROACH.
RHO(J)=RHO(N)+0.05
1 X=EXP(ALPHA*R)
Y=EXP(BETA*R)
Z=EXP(GAM*R)
XMP=1.008
XMT=39.948
ET=(0.5*(XMP*XMT)/(XMP+XMT))*EV(K)/XMP
V=(A*X+B*Y+C*Z)/ET
G=R**2-V*R-RHO(J)**2
DV=(A*ALPHA*X+B*BETA*Y+C*GAM*Z)/ET

```

```

H=V-R*DV+2.*RHO(J)**2./R
RNEW=R-G/H
D1FR=ABS((R-RNEW)/RNEW)
IF(D1FR-0.0001)4,2,2
2 ITN=ITN+1
3 IF(ITN-10000)3,7,7
R=RNEW
GO TO 1
4 CONTINUE
R=RNEW
V=(A*X+B*Y+C*Z)/ET
DV=(A*ALPHA*X+B*BETA*Y+C*GAM*Z)/ET
IF(R-RHO(J))7,120,61
THE NEXT 19 STEPS SOLVE FOR 'U', THE INTEGRAL USING A GAUSS
QUADRATURE FORMULA
61 QI=COS(3.14159/12.)
SJ=COS(3.14159/4.)
TK=COS(3.14159*5./12.)
QIA=EXP(ALPHA*R/QI)
QIB=EXP(BETA*R/QI)
QIC=EXP(GAM*R/QI)
VI=(A*QIA+B*QIB+C*QIC)/ET
GI=R/SQRT(R**2.-VI*R*QI-RHO(J)**2.*QI**2.)
SJA=EXP(ALPHA*R/SJ)
SJB=EXP(BETA*R/SJ)
SJC=EXP(GAM*R/SJ)
VJ=(A*SJA+B*SJB+C*SJC)/ET
GJ=R/SQRT(R**2.-VJ*R*SJ-RHO(J)**2.*SJ**2.)
TKA=EXP(ALPHA*R/TK)
TKB=EXP(BETA*R/TK)
TKC=EXP(GAM*R/TK)
VK=(A*TKA+B*TKB+C*TKC)/ET
GK=R/SQRT(R**2.-VK*R*TK-RHO(J)**2.*TK**2.)
U=(TK*GI+SJ*GJ+QI*GK)*3.14159/(6.*R)
THETA(J), THE SCATTERING ANGLE IN THE CM. IS NOW COMPUTED.
C
THE THETA(J)=3.14159-2.*RHO(J)*U
C
THE NEXT 14 STEPS SOLVE FOR DTHETA.
DGI=R*RHO(J)*QI**2./((SQRT(R**2.-VI*R*QI-RHO(J)**2.*QI**2.))**3
DGJ=R*RHO(J)*SJ**2./((SQRT(R**2.-VJ*R*SJ-RHO(J)**2.*SJ**2.))**3.
DGK=R*RHO(J)*TK**2./((SQRT(R**2.-VK*R*TK-RHO(J)**2.*TK**2.))**3
DU=3.14159*(TK*DGJ+SJ*DKG+QI*DKG)/(6.*R)
DRDRHO=2.*RHO(J)/(2.*RHO(J)**2./R-R*DV+V)
DVI=(A*ALPHA*QIA+B*BETA*QIB+C*GAM*QIC)/ET
DVJ=(A*ALPHA*SJA+B*BETA*SJB+C*GAM*SJC)/ET
DVK=(A*ALPHA*TKA+B*BETA*TKB+C*GAM*TKC)/ET
DGDRJ=(DVI/R-GI*VI/R**2.-2.*QI**2.*RHO(J)**2./R**3.)/(GI**3./2.)
DGDRJ=(DVJ/R-SJ*VJ/R**2.-2.*SJ**2.*RHO(J)**2./R**3.)/(GJ**3./2.)
DGDRK=(DVK/R-TK*VK/R**2.-2.*TK**2.*RHO(J)**2./R**3.)/(GK**3./2.)

```



```

DUDR=(TK*DGORI+SJ*DGDRJ+QI*DGDRK)*3.14159/(6.*R)-U/R
DUDRHO=DUDR*DRDRHO+DU
DTHEA=2.*U+2.*RHO(J)*DUDRHO
C   THE CROSS SECTION FOR H+ IS COMPUTED.
C   SIGMA=RHO(J)/(SIN(THETA(J))*DTHEA)
C   THETA IS CONVERTED TO LAB COORDINATES.
ARG= SIN(THETA(J))/((XMP/XMT)+COS(THETA(J)))
IF(ARG)41,41,42
41 ARG=100000
42 THETA(J)=ATAN(ARG)
204 DEG(J)=THETA(J)*180./3.14159
C   *RAD* IS THE EQUILIBRIUM SEPERATION IN UNITS OF BOHR RADII.
C   RAD=1.06/.529167
C   THE ORIENTATION PROBABILITY IS COMPUTED
P=8.*DENER*SIGMA/(3.14159*RAD*RAD*EV(K))
IF(P-1.)9,9,8
8 P=1
C   *CS* IS THE CROSS-SECTION OF H2+ CONVERTED TO CM.**2.
9 CS=SIGMA*P*(AO**2.)*10000.
SIGMA=SIGMA*(AO**2.)*10000.
IF(DEG(J)-90.)13,6,6
13 IF(DEG(J)-2.)6,6,12
12 WRITE(6,5)EV(K),RHO(J),R,DEG(J),SIGMA,P,CS
5 FORMAT(F8.2,2F12.3,F9.2,1P3E13.3)
6 CONTINUE
120 CONTINUE
15 CONTINUE
17 CONTINUE
END
RETURN
//GO.SYSIN DD *

```

## 2. Calculation of Ion Trajectory and Solid Angle.

As discussed in Section III E, the scattered ion trajectories and solid angles must be computed numerically. Since much of the computer program that accomplished this is peculiar to the Naval Postgraduate School IBM 360-67 computer installation, only an outline of the program is presented here.

Recall that the axial component of the magnetic field on the magnetic field axis was measured and expressed as a polynomial of the form

$$B_z(z, r = 0) = I \sum_{n=1}^{13} C_n z^{n-1}.$$

Bush [4] shows that a vector potential for this axially symmetric, non-uniform magnetic field can be written using this expression for  $B_z(z, r = 0)$  as:

$$A_\phi(r, z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n+1)!} \left(\frac{r}{2}\right)^{2n+1} \frac{\partial^{2n} B_z(z, r = 0)}{\partial z^{2n}}$$

$$A_r(r, z) = 0$$

$$A_z(r, z) = 0$$

Using this vector potential in the Lorentz force equation

$$\vec{F} = q \vec{v} \times \vec{B} = q \vec{v} \times (\vec{\nabla} \times \vec{A}),$$

it follows that:

$$F_r = m \left[ \frac{d^2 r}{dt^2} - r \left( \frac{d\phi}{dt} \right)^2 \right] = q \left[ \frac{d\phi}{dt} \frac{\partial (r A_\phi)}{\partial r} \right] \quad (1)$$

$$F_\phi = m \left[ 2 \left( \frac{dr}{dt} \right) \left( \frac{d\phi}{dt} \right) + r \frac{d^2 \phi}{dt^2} \right] = -q \left[ \left( \frac{dz}{dt} \right) \left( \frac{\partial A_\phi}{\partial z} \right) + \frac{1}{r} \frac{dr}{dz} \frac{\partial (r A_\phi)}{\partial r} \right] \quad (2)$$

$$F_z = m \left[ \frac{d^2 z}{dt^2} \right] = q \left[ r \frac{d\phi}{dt} \frac{\partial A_\phi}{\partial z} \right] \quad (3)$$

Equation (2) can be reduced to  $\frac{d\phi}{dt} = -q \frac{A_\phi}{mr}$ . Using this, equations (1) and (3) can be combined to eliminate the time dependence to

$$\frac{\frac{d^2 r}{dz^2}}{\left[1 + \left(\frac{dr}{dz}\right)^2\right]} \left[ \frac{p^2}{q} - A_\phi^2 \right] - \frac{dr}{dz} \left[ A_\phi \frac{\partial A_\phi}{\partial z} \right] + A_\phi \frac{\partial A_\phi}{\partial r} = 0. \quad (4)$$

This is a second-order, non-linear differential equation whose solution describes the trajectory of the scattered ion in the magnetic field. In order to integrate it numerically, it is expressed as two first-order, simultaneous differential equations as follows.

$$\text{Let } y_1 = r$$

$$y_2 = \frac{dr}{dz} = \frac{dy_1}{dz}$$

$$f_1 = \frac{A_\phi \frac{\partial A_\phi}{\partial z}}{\frac{p^2}{q} - A_\phi^2}$$

$$f_2 = \frac{A_\phi \frac{\partial A_\phi}{\partial r}}{\frac{p^2}{q} - A_\phi^2}$$

Then equation (4) may be equivalently written as

$$\frac{dy_1}{dz} = y_2 \quad (5)$$

$$\frac{dy_2}{dz} = f_1 y_2^3 - f_2 y_2^2 + f_1 y_2 - f_2 \quad (6)$$

Equations (5) and (6) were integrated by the DHPGC subroutine which employs a Hamming's modified predictor-corrector method. The solution to (5) and (6) yields the trajectory and hence  $Z_0$  and  $\theta_0$ . Now in a single computer run, the trajectory equations were solved a number of times for various scattering angles. Typically this would be for  $\theta$  from  $35^\circ$  to  $55^\circ$  in  $1^\circ$  increments. A second subroutine was then called on to generate a seventh order least squares polynomial fit of  $\theta = f(Z_0)$ . From  $\theta_0$  and the detector geometry,  $\Delta Z_0$  was computed. The solid angle could then be computed by the expression

$$d\Omega \approx 2\pi \left( \frac{290}{360} \right) \sin \theta \left| \frac{\partial \theta}{\partial Z_0} \right| \Delta Z_0 .$$

The computer output then tabulated  $\theta$ ,  $Z_0$ ,  $\Delta Z_0$ ,  $\theta_0$ , and  $d\Omega$  as well as a plot of the trajectory (see Fig. 12) if desired.

## LIST OF REFERENCES

1. Feist, P.E. Classical Calculation of the Differential Cross Section for Scattering of Hydrogen Molecular Ions From Heavy Atoms, Master's Thesis, Naval Postgraduate School, Monterey, California, June 1967.
2. Bates, D.R., Cook, C.J., and Smith, F.J., "Classical Theory of Ion-Molecule Rearrangement Collisions at High Impact Energies," Proceedings of the Physical Society, V. 83, p. 49-57, (1964).
3. Byatt, W.J., "Analytical Representation of Hartree Potentials and Electron Scattering," The Physical Review, V. 104, p. 1298-1300, 1 December (1956).
4. Bush, T.O. Large Angle Scattering of Lithium Ions by Helium Atoms, Ph.D. Thesis, Naval Postgraduate School, Monterey, California, September 1968.
5. Carter, T.L., Ion Sources for the Production of Low Energy Beams, Master's Thesis, Naval Postgraduate School, Monterey, California, June 1968.
6. Strohsahl, G.H., Jr., Construction and Calibration of a Mass Spectrometer for the Analysis of Light Ions, Master's Thesis, Naval Postgraduate School, Monterey, California, December, 1967.
7. Kelly, P.J., Analogue Measurements of Charged Particle Trajectories in an Inhomogeneous Magnetic Field, Master's Thesis, Naval Postgraduate School, Monterey, California, 1965.
8. Bush, T.O., Cook, C.J., Heinz, O., and Rodeback, G.W., "Measurement of Large Angle Atomic Scattering Using Axially Symmetric Magnetic Fields," Paper submitted for publication, 1969.
9. Boring, J.W., Magnuson, G.D., and Snyder, R.S., "Elastic Differential Scattering of  $H^+$ ,  $He^+$ , and  $Ne^{++}$  by Ar," paper presented at meeting of the American Physical Society, February 1969, St. Louis, Mo. Also private communication in August 1969.
10. Smith, F.T., Marchi, R.P., Aberth, W., Lorents, D.C., and Heinz, O., "Collision Spectroscopy. I. Analysis of the Scattering of  $He^+$  by Ne and Ar," The Physical Review, V. 161, p. 31-46, 5 September (1967).
11. Aberth, W., and Lorents, C.L., "Elastic Differential Scattering of  $He^+$  Ions by Neon and Ar and of  $Ar^+$  by Ar in the 10-600 eV. Range," The Physical Review, V. 144, p. 109-115, 8 April (1966).



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<p>The elastic differential scattering cross sections for <math>H^+, H_2^+ + Ar \rightarrow H^+, H_2^+ + Ar</math> were measured for angles of <math>39^\circ</math> to <math>50^\circ</math> with incident lab energy of 100 eV. The apparatus utilized the properties of axially symmetric, non-uniform magnetic fields (large thin solenoid) to focus all scattered ions with vector momentum <math>\vec{p}</math> within <math>\Delta\vec{p}</math> onto a detector placed down the magnetic axis. Thus, the solid angle was increased by a factor of about 300 over conventional methods with comparable resolution in <math>\Delta\theta</math> (about <math>1^\circ</math>). A typical value for <math>\sigma_{H^+}(43^\circ)</math> is <math>8.2 \times 10^{-18} \text{ cm}^2</math>. The <math>H^+</math> data was compared with data of Magnuson, et.al., via a scaling law and was in excellent agreement. A typical value for <math>\sigma_{H_2^+}(43^\circ)</math> is <math>2.4 \times 10^{-20} \text{ cm}^2</math>. A simple refinement of a classical model for <math>H_2^+</math> scattering by Feist relates these cross sections by <math>\sigma_{H_2^+}(\theta) = P \sigma_{H^+}(\theta)</math></p> $\sim \frac{4D}{\pi l^2 E_0} [\sigma_{H^+}(\theta)]^2$ <p>where P is an orientation factor, D the binding energy, and l the internuclear separation. This expression relates the cross sections to within the accuracy of the experiment thus verifying the classical approximations.</p>			

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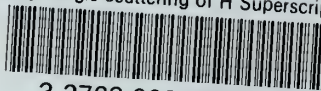






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